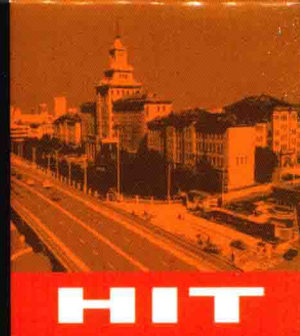


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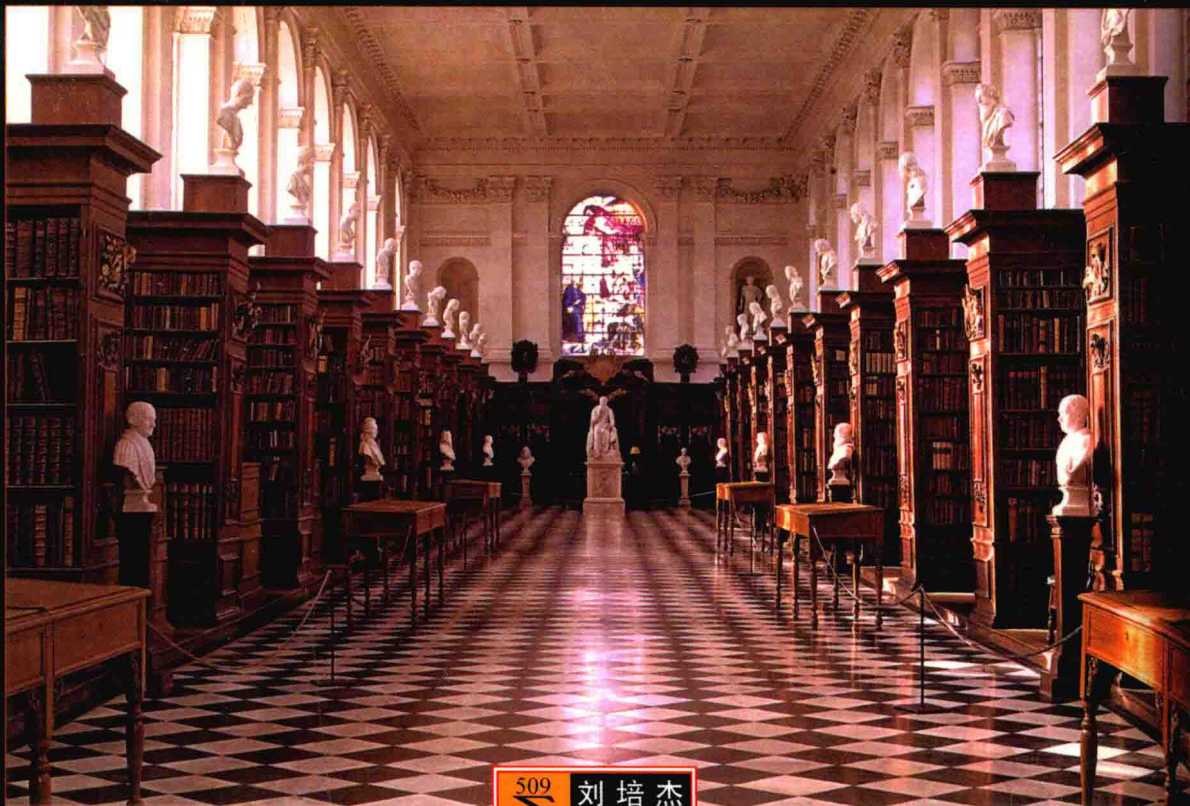
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Francoise, J. P. (弗朗索瓦斯) Naber, G. L. (纳伯) Tsou Sheung Tsun (孙圣周) 著



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FOREWORD

In bygone centuries, our physical world appeared to be filled to the brim with mysteries. Divine powers could provide for genuine miracles; water and sunlight could turn arid land into fertile pastures, but the same powers could lead to miseries and disasters. The force of life, the *vis vitalis*, was assumed to be the special agent responsible for all living things. The heavens, whatever they were for, contained stars and other heavenly bodies that were the exclusive domain of the Gods.

Mathematics did exist, of course. Indeed, there was one aspect of our physical world that was recognised to be controlled by precise, mathematical logic: the geometric structure of space, elaborated to become a genuine form of art by the ancient Greeks. From my perspective, the Greeks were the first practitioners of ‘mathematical physics’, when they discovered that all geometric features of space could be reduced to a small number of axioms. Today, these would be called ‘fundamental laws of physics’. The fact that the flow of *time* could be addressed with similar exactitude, and that it could be handled geometrically together with space, was only recognised much later. And, yes, there were a few crazy people who were interested in the magic of numbers, but the real world around us seemed to contain so much more that was way beyond our capacities of analysis.

Gradually, all this changed. The Moon and the planets appeared to follow geometrical laws. Galilei and Newton managed to identify their logical rules of motion, and by noting that the concept of mass could be applied to things in the sky just like apples and cannon balls on Earth, they made the sky a little bit more accessible to us. Electricity, magnetism, light and sound were also found to behave in complete accordance with mathematical equations.

Yet all of this was just a beginning. The real changes came with the twentieth century. A completely new way of thinking, by emphasizing mathematical, logical analysis rather than empirical evidence, was pioneered by Albert Einstein. Applying advanced mathematical concepts, only known to a few pure mathematicians, to notions as mundane as space and time, was new to the physicists of his time. Einstein himself had a hard time struggling through the logic of connections and curvatures, notions that were totally new to him, but are only too familiar to students of mathematical physics today. Indeed, there is no better testimony of Einstein’s deep insights at that time, than the fact that we now teach these things regularly in our university classrooms.

Special and general relativity are only small corners of the realm of modern physics that is presently being studied using advanced mathematical methods. We have notoriously complex subjects such as phase transitions in condensed matter physics, superconductivity, Bose–Einstein condensation, the quantum Hall effect, particularly the fractional quantum Hall effect, and numerous topics from elementary particle physics, ranging from fibre bundles and renormalization groups to supergravity, algebraic topology, superstring theory, Calabi–Yau spaces and what not, all of which require the utmost of our mental skills to comprehend them.

The most bewildering observation that we make today is that it seems that our *entire* physical world appears to be controlled by mathematical equations, and these are not just sloppy and debatable models, but precisely documented properties of materials, of systems, and of phenomena in all echelons of our universe.

Does this really apply to our entire world, or only to parts of it? Do features, notions, entities exist that are emphatically *not* mathematical? What about intuition, or dreams, and what about consciousness? What about religion? Here, most of us would say, one should not even try to apply mathematical analysis, although even here, some brave social scientists are making attempts at coordinating rational approaches.

No, there are clear and important differences between the physical world and the mathematical world. Where the physical world stands out is the fact that it refers to ‘reality’, whatever ‘reality’ is. Mathematics is the world of pure logic and pure reasoning. In physics, it is the experimental evidence that ultimately decides whether a theory is acceptable or not. Also, the methodology in physics is different.

A beautiful example is the serendipitous discovery of superconductivity. In 1911, the Dutch physicist Heike Kamerlingh Onnes was the first to achieve the liquefaction of helium, for which a temperature below 4.25 K had to be realized. Heike decided to measure the specific conductivity of mercury, a metal that is frozen solid at such low temperatures. But something appeared to go wrong during the measurements, since the volt meter did not show any voltage at all. All experienced physicists in the team assumed that they were dealing with a malfunction. It would not have been the first time for a short circuit to occur in the electrical equipment, but, this time, in spite of several efforts, they failed to locate it. One of the assistants was responsible for keeping the temperature of the sample well within that of liquid helium, a dull job, requiring nothing else than continuously watching some dials. During one of the many tests, however, he dozed off. The temperature rose, and suddenly the measurements showed the normal values again. It then occurred to the investigators that the effect and its temperature dependence were completely reproducible. Below 4.19 degrees Kelvin the conductivity of mercury appeared to be strictly infinite. Above that temperature, it is finite, and the transition is a very sudden one. Superconductivity was discovered (D. van Delft, “Heike Kamerling Onnes”, Uitgeverij Bert Bakker, Amsterdam, 2005 (in Dutch)).

This is not the way mathematical discoveries are made. Theorems are not produced by assistants falling asleep, even if examples do exist of incidents involving some miraculous fortune.

The hybrid science of mathematical physics is a very curious one. Some of the topics in this Encyclopedia are undoubtedly physical. High T_c superconductivity, breaking water waves, and magneto-hydrodynamics, are definitely topics of physics where experimental data are considered more decisive than any high-brow theory. Cohomology theory, Donaldson–Witten theory, and AdS/CFT correspondence, however, are examples of purely mathematical exercises, even if these subjects, like all of the others in this compilation, are strongly inspired by, and related to, questions posed in physics.

It is inevitable, in a compilation of a large number of short articles with many different authors, to see quite a bit of variation in style and level. In this Encyclopedia, theoretical physicists as well as mathematicians together made a huge effort to present in a concise and understandable manner their vision on numerous important issues in advanced mathematical physics. All include references for further reading. We hope and expect that these efforts will serve a good purpose.

Gerard 't Hooft,
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PREFACE

Mathematical Physics as a distinct discipline is relatively new. The International Association of Mathematical Physics was founded only in 1976. The interaction between physics and mathematics has, of course, existed since ancient times, but the recent decades, perhaps partly because we are living through them, appear to have witnessed tremendous progress, yielding new results and insights at a dizzying pace, so much so that an encyclopedia seems now needed to collate the gathered knowledge.

Mathematical Physics brings together the two great disciplines of Mathematics and Physics to the benefit of both, the relationship between them being symbiotic. On the one hand, it uses mathematics as a tool to organize physical ideas of increasing precision and complexity, and on the other it draws on the questions that physicists pose as a source of inspiration to mathematicians. A classical example of this relationship exists in Einstein's theory of relativity, where differential geometry played an essential role in the formulation of the physical theory while the problems raised by the ensuing physics have in turn boosted the development of differential geometry. It is indeed a happy coincidence that we are writing now a preface to an encyclopedia of mathematical physics in the centenary of Einstein's *annus mirabilis*.

The project of putting together an encyclopedia of mathematical physics looked, and still looks, to us a formidable enterprise. We would never have had the courage to undertake such a task if we did not believe, first, that it is worthwhile and of benefit to the community, and second, that we would get the much-needed support from our colleagues. And this support we did get, in the form of advice, encouragement, and practical help too, from members of our Editorial Advisory Board, from our authors, and from others as well, who have given unstintingly so much of their time to help us shape this Encyclopedia.

Mathematical Physics being a relatively new subject, it is not yet clearly delineated and could mean different things to different people. In our choice of topics, we were guided in part by the programs of recent International Congresses on Mathematical Physics, but mainly by the advice from our Editorial Advisory Board and from our authors. The limitations of space and time, as well as our own limitations, necessitated the omission of certain topics, but we have tried to include all that we believe to be core subjects and to cover as much as possible the most active areas.

Our subject being interdisciplinary, we think it appropriate that the Encyclopedia should have certain special features. Applications of the same mathematical theory, for instance, to different problems in physics will have different emphasis and treatment. By the same token, the same problem in physics can draw upon resources from different mathematical fields. This is why we divide the Encyclopedia into two broad sections: physics subjects and related mathematical subjects. Articles in either section are deliberately allowed a fair amount of overlap with one another and many articles will appear under more than one heading, but all are linked together by elaborate cross referencing. We think this gives a better picture of the subject as a whole and will serve better a community of researchers from widely scattered yet related fields.

The Encyclopedia is intended primarily for experienced researchers but should be of use also to beginning graduate students. For the latter category of readers, we have included eight elementary introductory articles for easy reference, with those on mathematics aimed at physics graduates and those on physics aimed at mathematics graduates, so that these articles can serve as their first port of call to enable them to embark on any of the main articles without the need to consult other material beforehand. In fact, we think these articles may even form the

foundation of advanced undergraduate courses, as we know that some authors have already made such use of them.

In addition to the printed version, an on-line version of the Encyclopedia is planned, which will allow both the contents and the articles themselves to be updated if and when the occasion arises. This is probably a necessary provision in such a rapidly advancing field.

This project was some four years in the making. Our foremost thanks at its completion go to the members of our Editorial Advisory Board, who have advised, helped and encouraged us all along, and to all our authors who have so generously devoted so much of their time to writing these articles and given us much useful advice as well. We ourselves have learnt a lot from these colleagues, and made some wonderful contacts with some among them. Special thanks are due also to Arthur Greenspoon whose technical expertise was indispensable.

The project was started with Academic Press, which was later taken over by Elsevier. We thank warmly members of their staff who have made this transition admirably seamless and gone on to assist us greatly in our task: both Carey Chapman and Anne Guillaume, who were in charge of the whole project and have been with us since the beginning, and Edward Taylor responsible for the copy-editing. And Martin Ruck, who manages to keep an overwhelming amount of details constantly at his fingertips, and who is never known to have lost a single email, deserves a very special mention.

As a postscript, we would like to express our gratitude to the very large number of authors who generously agreed to donate their honorariums to support the Committee for Developing Countries of the European Mathematical Society in their work to help our less fortunate colleagues in the developing world.

Jean-Pierre Francoise
Gregory L. Naber
Tsou Sheung Tsun

GUIDE TO USE OF THE ENCYCLOPEDIA

Structure of the Encyclopedia

The material in this Encyclopedia is organised into two sections. At the start of Volume 1 are eight **Introductory Articles**. The introductory articles on mathematics are aimed at physics graduates; those on physics are aimed at mathematics graduates. It is intended that these articles should serve as the first port of call for graduate students, to enable them to embark on any of the main entries without the need to consult other material beforehand.

Following the Introductory Articles, the main body of the Encyclopedia is arranged as a series of entries in alphabetical order. These entries fill the remainder of Volume 1 and all of the subsequent volumes (2–5).

To help you realize the full potential of the material in the Encyclopedia we have provided four features to help you find the topic of your choice: a contents list by subject, an alphabetical contents list, cross-references, and a full subject index.

1. Contents List by Subject

Your first point of reference will probably be the contents list by subject. This list appears at the front of each volume, and groups the entries under subject headings describing the broad themes of mathematical physics. This will enable the reader to make quick connections between entries and to locate the entry of interest. The contents list by subject is divided into two main sections: *Physics Subjects* and *Related Mathematics Subjects*. Under each main section heading, you will find several subject areas (such as GENERAL RELATIVITY in Physics Subjects or NONCOMMUTATIVE GEOMETRY in Related Mathematics Subjects). Under each subject area is a list of those entries that cover aspects of that subject, together with the volume and page numbers on which these entries may be found.

Because mathematical physics is so highly interconnected, individual entries may appear under more than one subject area. For example, the entry GAUGE THEORY: MATHEMATICAL APPLICATIONS is listed under the Physics Subject GAUGE THEORY as well as in a broad range of Related Mathematics Subjects.

2. Alphabetical Contents List

The alphabetical contents list, which also appears at the front of each volume, lists the entries in the order in which they appear in the Encyclopedia. This list provides both the volume number and the page number of the entry.

You will find “dummy entries” where obvious synonyms exist for entries or where we have grouped together related topics. Dummy entries appear in both the contents list and the body of the text.

Example

If you were attempting to locate material on path integral methods via the alphabetical contents list:

PATH INTEGRAL METHODS *see* Functional Integration in Quantum Physics; Feynman Path Integrals

The dummy entry directs you to two other entries in which path integral methods are covered. At the appropriate locations in the contents list, the volume and page numbers for these entries are given.

If you were trying to locate the material by browsing through the text and you had looked up Path Integral Methods, then the following information would be provided in the dummy entry:

Path Integral Methods <i>see</i> Functional Integration in Quantum Physics; Feynman Path Integrals

3. Cross-References

All of the articles in the Encyclopedia have been extensively cross-referenced. The cross-references, which appear at the end of an entry, serve three different functions:

- i. To indicate if a topic is discussed in greater detail elsewhere.
- ii. To draw the reader's attention to parallel discussions in other entries.
- iii. To indicate material that broadens the discussion.

Example

The following list of cross-references appears at the end of the entry STOCHASTIC HYDRODYNAMICS

See also: Cauchy Problem for Burgers-Type Equations; Hamiltonian Fluid Dynamics; Incompressible Euler Equations: Mathematical Theory; Malliavin Calculus; Non-Newtonian Fluids; Partial Differential Equations: Some Examples; Stochastic Differential Equations; Turbulence Theories; Viscous Incompressible Fluids: Mathematical Theory; Vortex Dynamics

Here you will find examples of all three functions of the cross-reference list: a topic discussed in greater detail elsewhere (e.g. Incompressible Euler Equations: Mathematical Theory), parallel discussion in other entries (e.g. Stochastic Differential Equations) and reference to entries that broaden the discussion (e.g. Turbulence Theories).

The eight Introductory Articles are not cross-referenced from any of the main entries, as it is expected that introductory articles will be of general interest. As mentioned above, the Introductory Articles may be found at the start of Volume 1.

4. Index

The index will provide you with the volume and page number where the material is located. The index entries differentiate between material that is a whole entry, is part of an entry, or is data presented in a figure or table. Detailed notes are provided on the opening page of the index.

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D

Deformation Quantization

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Introduction

Deformation quantization is an alternative way of looking at quantum mechanics. Some of its techniques were introduced by the pioneers of quantum mechanics, but it was first proposed as an autonomous theory in a paper in *Annals of Physics* (Bayen *et al.* 1978). More recent reviews treat modern developments (HH I 2001, Dito and Sternheimer 2002, Zachos 2002).

Deformation quantization concentrates on the central physical concepts of quantum theory: the algebra of observables and their dynamical evolution. Because it deals exclusively with functions of phase-space variables, its conceptual break with classical mechanics is less severe than in other approaches. It formulates the correspondence principle very precisely which played such an important role in the historical development.

Although this article deals mainly with nonrelativistic bosonic systems, deformation quantization is much more general. For inclusion of fermions and the Dirac equation see (Hirshfeld *et al.* 2002b). The fermionic degrees of freedom may, in special cases, be obtained from the bosonic ones by supersymmetric extension (Hirshfeld *et al.* 2004). For applications to field theory, see Hirshfeld *et al.* (2002). For the relation to Hopf algebras see Hirshfeld *et al.* (2003), and to geometric algebra, see Hirshfeld *et al.* (2005).

The observables of a physical system, such as the Hamilton function, are smooth real-valued functions on phase space. Physical quantities of the system at some time, such as the energy, are calculated by evaluating the Hamilton function at the point $x_0 = (q_0, p_0)$ in phase space that characterizes the state of the system at this time (we assume for the moment, a one-particle system). The mathematical expression for this operation is

$$E = \int H(q, p) \delta^{(2)}(q - q_0, p - p_0) dq dp \quad [1]$$

where $\delta^{(2)}$ is the two-dimensional Dirac delta function. The observables of the dynamical system are functions on the phase space, the states of the system are positive functionals on the observables (here the Dirac delta functions), and we obtain the value of the observable in a definite state by the operation shown in eqn [1].

In general, functions on a manifold are multiplied by each other in a pointwise manner, that is, given two functions f and g , their product fg is the function

$$(fg)(x) = f(x)g(x) \quad [2]$$

In the context of classical mechanics, the observables build a commutative algebra, called the commutative “classical algebra of observables.”

In Hamiltonian mechanics there is another way to combine two functions on phase space in such a way that the result is again a function on the phase space, namely by using the Poisson bracket

$$\begin{aligned} \{f, g\}(q, p) &= \sum_{i=1}^n \left(\frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i} \right) \Big|_{q, p} \\ &= f \left(\overleftarrow{\partial}_q \overleftarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_q \right) g \end{aligned} \quad [3]$$

in an abbreviated notation.

The notation can be further abbreviated by using x to represent points of the phase-space manifold, $x = (x_1, \dots, x_{2n})$, and introducing the Poisson tensor α^{ij} , where the indices i, j run from 1 to $2n$. In canonical coordinates α^{ij} is represented by the matrix

$$\alpha = \begin{pmatrix} 0 & -I_n \\ I_n & 0 \end{pmatrix} \quad [4]$$

where I_n is the $n \times n$ identity matrix. Then eqn [3] becomes

$$\{f, g\}(x) = \alpha^{ij} \partial_i f(x) \partial_j g(x) \quad [5]$$

where $\partial_i = \partial/\partial x_i$.

For a general observable,

$$\dot{f} = \{f, H\} \quad [6]$$

Because α transforms like a tensor with respect to coordinate transformations, eqn [5] may also be written in noncanonical coordinates. In this case the components of α need not be constants, and may depend on the point of the manifold at which they are evaluated. But in Hamiltonian mechanics, α is still required to be invertible. A manifold equipped with a Poisson tensor of this kind is called a symplectic manifold. In general, the tensor α is no longer required to be invertible, but it nevertheless suffices to define Poisson brackets via eqn [5], and these brackets are required to have the properties

1. $\{f, g\} = -\{g, f\}$,
2. $\{f, gh\} = \{f, g\}h + g\{f, h\}$, and
3. $\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0$.

Property (1) implies that the Poisson bracket is antisymmetric, property (2) is referred to as the Leibnitz rule, and property (3) is called the Jacobi identity. The Poisson bracket used in Hamiltonian mechanics satisfies all these properties, but we now abstract these properties from the concrete prescription of eqn [3], and a Poisson manifold (M, α) is defined as a smooth manifold M equipped with a Poisson tensor α , whose components are no longer necessarily constant, such that the bracket defined by eqn [5] has the above properties. It turns out that such manifolds provide a better context for treating dynamical systems with symmetries. In fact, they are essential for treating gauge-field theories, which govern the fundamental interactions of elementary particles.

Quantum Mechanics and Star Products

The essential difference between classical and quantum mechanics is Heisenberg's uncertainty relation, which implies that in the latter, states can no longer be represented as points in phase space. The uncertainty is a consequence of the noncommutativity of the quantum mechanical observables. That is, the commutative classical algebra of observables must be replaced by a noncommutative quantum algebra of observables.

In the conventional approach to quantum mechanics, this noncommutativity is implemented by representing the quantum mechanical observables by linear operators in Hilbert space. Physical quantities are then represented by eigenvalues of these operators, and physical states are related to the operator eigenfunctions. Although these entities are somehow related to their classical counterparts, to which they are supposed to reduce in an appropriate limit, the precise relationship has remained obscure, one hundred years after the beginnings of quantum

mechanics. Textbooks refer to the correspondence principle, which guided the pioneers of the subject. Attempts to give this idea a precise formulation by postulating a specific relation between the classical Poisson brackets of observables and the commutators of the corresponding quantum mechanical operators, as undertaken, for example, by Dirac and von Neumann, encountered insurmountable difficulties, as pointed out by Groenewold in 1946 in an unjustly neglected paper (Groenewold 1948). In the same paper Groenewold also wrote down the first explicit representation of a "star product" (see eqn [11]), without however realizing the potential of this concept for overcoming the difficulties that he wanted to resolve.

In the deformation quantization approach, there is no such break when going from the classical system to the corresponding quantum system; we describe the quantum system by using the same entities that are used to describe the classical system. The observables of the system are described by the same functions on phase space as their classical counterparts. Uncertainty is realized by describing physical states as distributions on phase space that are not sharply localized, in contrast to the Dirac delta functions which occur in the classical case. When we evaluate an observable in some definite state according to the quantum analog of eqn [1] (see eqn [24]), values of the observable in a whole region contribute to the number that is obtained, which is thus an average value of the observable in the given state. Noncommutativity is incorporated by introducing a noncommutative product for functions on phase space, so that we get a new noncommutative quantum algebra of observables. The systematic work on deformation quantization stems from Gerstenhaber's seminal paper, where he introduced the concept of a star product of smooth functions on a manifold (Gerstenhaber 1964).

For applications to quantum mechanics, we consider smooth complex-valued functions on a Poisson manifold. A star product $f * g$ of two such functions is a new smooth function, which, in general, is described by an infinite power series:

$$\begin{aligned} f * g &= fg + (i\hbar)C_1(f, g) + O(\hbar^2) \\ &= \sum_{n=0}^{\infty} (i\hbar)^n C_n(f, g) \end{aligned} \quad [7]$$

The first term in the series is the pointwise product given in eqn [2], and $(i\hbar)$ is the deformation parameter, which is assumed to be varying continuously. If \hbar is identified with Planck's constant, then what varies is really the magnitude of the

action of the dynamical system considered in units of \hbar : the classical limit holds for systems with large action. In this limit, which we express here as $\hbar \rightarrow 0$, the star product reduces to the usual product. In general, the coefficients C_n will be such that the new product is noncommutative, and we consider the noncommutative algebra formed from the functions with this new multiplication law as a deformation of the original commutative algebra, which uses pointwise multiplication of the functions.

The expressions $C_n(f, g)$ denote functions made up of the derivatives of the functions f and g . It is obvious that without further restrictions of these coefficients, the star product is too arbitrary to be of any use. Gerstenhaber's discovery was that the simple requirement that the new product be associative imposes such strong requirements on the coefficients C_n that they are essentially unique in the most important cases (up to an equivalence relation, as discussed below). Formally, Gerstenhaber required that the coefficients satisfy the following properties:

1. $\sum_{j+k=n} C_j(C_k(f, g), h) = \sum_{j+k=n} C_j(f, C_k(g, h))$,
2. $C_0(f, g) = fg$, and
3. $C_1(f, g) - C_1(g, f) = \{f, g\}$.

Property (1) guarantees that the star product is associative: $(f * g) * h = f * (g * h)$. Property (2) means that in the limit $\hbar \rightarrow 0$, the star product $f * g$ agrees with the pointwise product fg . Property (3) has at least two aspects: (i) mathematically, it anchors the new product to the given structure of the Poisson manifold and (ii) physically, it provides the connection between the classical and quantum behavior of the dynamical system. Define a commutator by using the new product:

$$[f, g]_* = f * g - g * f \quad [8]$$

Property (3) may then be written as

$$\lim_{\hbar \rightarrow 0} \frac{1}{i\hbar} [f, g]_* = \{f, g\} \quad [9]$$

Equation [9] is the correct form of the correspondence principle. In general, the quantity on the left-hand side of eqn [9] reduces to the Poisson bracket only in the classical limit. The source of the mathematical difficulties that previous attempts to formulate the correspondence principle encountered was related to trying to enforce equality between the Poisson bracket and the corresponding expression involving the quantum mechanical commutator. Equation [9] shows that such a relation in general only holds up to corrections of higher order in \hbar .

For physical applications we usually require the star product to be Hermitean: $\overline{f * g} = \bar{g} * \bar{f}$, where \bar{f} denotes the complex conjugate of f . The star products considered in this article have this property.

For a given Poisson manifold, it is not clear *a priori* if a star product for the smooth functions on the manifold actually exists, that is, whether it is at all possible to find coefficients C_n that satisfy the above list of properties. Even if we find such coefficients, it is still not clear that the series they define through eqn [7] yields a smooth function. Mathematicians have worked hard to answer these questions in the general case. For flat Euclidian spaces, $M = \mathbb{R}^{2n}$, a specific star product has long been known. In this case, the components of the Poisson tensor α^{ij} can be taken to be constants. The coefficient C_1 can then be chosen antisymmetric, so that

$$C_1(f, g) = \frac{1}{2} \alpha^{ij} (\partial_i f) (\partial_j g) = \frac{1}{2} \{f, g\} \quad [10]$$

by property (3) above. The higher-order coefficients may be obtained by exponentiation of C_1 . This procedure yields the Moyal star product (Moyal 1949):

$$f *_M g = f \exp \left(\left(\frac{i\hbar}{2} \right) \alpha^{ij} \overleftarrow{\partial}_i \overrightarrow{\partial}_j \right) g \quad [11]$$

In canonical coordinates, eqn [11] becomes

$$(f *_M g)(q, p) = f(q, p) \exp \left(\frac{i\hbar}{2} (\overleftarrow{\partial}_q \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_q) \right) g(q, p) \quad [12]$$

$$= \sum_{m,n=0}^{\infty} \left(\frac{i\hbar}{2} \right)^{m+n} \frac{(-1)^m}{m!n!} (\partial_p^m \partial_q^n f) (\partial_p^n \partial_q^m g) \quad [13]$$

We now come to the question of uniqueness of the star product on a given Poisson manifold. Two star products $*$ and $*$ ' are said to be "*c*-equivalent" if there exists an invertible transition operator

$$T = 1 + \hbar T_1 + \dots = \sum_{n=0}^{\infty} \hbar^n T_n \quad [14]$$

where the T_n are differential operators that satisfy

$$f *' g = T^{-1}((Tf) * (Tg)) \quad [15]$$

It is known that for $M = \mathbb{R}^{2n}$ all admissible star products are *c*-equivalent to the Moyal product. The concept of *c*-equivalence is a mathematical one (*c* stands for cohomology (Gerstenhaber 1964)); it does not by itself imply any kind of physical equivalence, as shown below.

Another expression for the Moyal product is a kind of Fourier representation:

$$\begin{aligned} (f *_{\text{M}} g)(q, p) &= \frac{1}{\hbar^2 \pi^2} \int dq_1 dq_2 dp_1 dp_2 f(q_1, p_1) g(q_2, p_2) \\ &\quad \times \exp \left[\frac{2}{i\hbar} (p(q_1 - q_2) + q(p_2 - p_1) \right. \\ &\quad \left. + (q_2 p_1 - q_1 p_2)) \right] \end{aligned} \quad [16]$$

Equation [16] has an interesting geometrical interpretation. Denote points in phase space by vectors, for example, in two dimensions:

$$\mathbf{r} = \begin{pmatrix} q \\ p \end{pmatrix}, \quad \mathbf{r}_1 = \begin{pmatrix} q_1 \\ p_1 \end{pmatrix}, \quad \mathbf{r}_2 = \begin{pmatrix} q_2 \\ p_2 \end{pmatrix} \quad [17]$$

Now, consider the triangle in phase space spanned by the vectors $\mathbf{r} - \mathbf{r}_1$ and $\mathbf{r} - \mathbf{r}_2$. Its area (symplectic volume) is

$$\begin{aligned} A(\mathbf{r}, \mathbf{r}_1, \mathbf{r}_2) &= \frac{1}{2} (\mathbf{r} - \mathbf{r}_1) \wedge (\mathbf{r} - \mathbf{r}_2) \\ &= \frac{1}{2} [p(q_2 - q_1) + q(p_1 - p_2) + (q_1 p_2 - q_2 p_1)] \end{aligned} \quad [18]$$

which is proportional to the exponent in eqn [16]. Hence, we may rewrite eqn [16] as

$$\begin{aligned} (f * g)(\mathbf{r}) &= \int d\mathbf{r}_1 d\mathbf{r}_2 f(\mathbf{r}_1) g(\mathbf{r}_2) \exp \left[\frac{4i}{\hbar} A(\mathbf{r}, \mathbf{r}_1, \mathbf{r}_2) \right] \end{aligned} \quad [19]$$

Deformation Quantization

The properties of the star product are well adapted for describing the noncommutative quantum algebra of observables. We have already discussed the associativity and the incorporation of the classical and semiclassical limits. Note that the characteristic nonlocality feature of quantum mechanics is also explicit. In the expression for the Moyal product given in eqn [13], the star product of the functions f and g at the point $x = (q, p)$ involves not only the values of the functions f and g at this point, but also all higher derivatives of these functions at x . But for a smooth function, knowledge of all the derivatives at a given point is equivalent to the knowledge of the function on the entire space. In the integral expression of eqn [16], we also see that knowledge of the functions f and g on the whole phase space is necessary to determine the value of the star product at the point x .

The c -equivalent star products correspond to different quantization schemes. Having chosen a quantization scheme, the quantities of interest for the quantum system may be calculated. It turns out that different quantization schemes lead to different spectra for the observables. The choice of a specific quantization scheme can only be motivated by further physical requirements. In the simple example we discuss below, the classical system is completely specified by its Hamilton function. In more general cases, one may have to decide what constitutes a sufficiently large set of good observables for a complete specification of the system (Bayen *et al.* 1978).

A state is characterized by its energy E ; the set of all possible values for the energy is called the spectrum of the system. The states are described by distributions on phase space called projectors. The state corresponding to the energy E is denoted by $\pi_E(q, p)$. These distributions are normalized:

$$\frac{1}{2\pi\hbar} \int \pi_E(q, p) dq dp = 1 \quad [20]$$

and idempotent:

$$(\pi_E * \pi_{E'})(q, p) = \delta_{E,E'} \pi_E(q, p) \quad [21]$$

The fact that the Hamilton function takes the value E when the system is in the state corresponding to this energy is expressed by the equation

$$(H * \pi_E)(q, p) = E \pi_E(q, p) \quad [22]$$

Equation [22] corresponds to the time-independent Schrödinger equation, and is sometimes called the “*-genvalue equation.” The spectral decomposition of the Hamilton function is given by

$$H(q, p) = \sum_E E \pi_E(q, p) \quad [23]$$

where the summation sign may indicate an integration if the spectrum is continuous. The quantum mechanical version of eqn [1] is

$$\begin{aligned} E &= \frac{1}{2\pi\hbar} \int (H * \pi_E)(q, p) dq dp \\ &= \frac{1}{2\pi\hbar} \int H(q, p) \pi_E(q, p) dq dp \end{aligned} \quad [24]$$

where the last expression may be obtained by using eqn [16] for the star product.

The time-evolution function for a time-independent Hamilton function is denoted by $\text{Exp}(Ht)$, and the fact that the Hamilton function is the generator of the time evolution of the system is expressed by

$$i\hbar \frac{d}{dt} \text{Exp}(Ht) = H * \text{Exp}(Ht) \quad [25]$$

This equation corresponds to the time-dependent Schrödinger equation. It is solved by the star exponential:

$$\text{Exp}(Ht) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{-it}{\hbar} \right)^n (H*)^n \quad [26]$$

where $(H*)^n = \underbrace{H*H*\dots*H}_{n \text{ times}}$. Because each state of definite energy E has a time evolution $\exp(iEt/\hbar)$, the complete time-evolution function may be written in the form

$$\text{Exp}(Ht) = \sum_E \pi_E e^{-iEt/\hbar} \quad [27]$$

This expression is called the “Fourier–Dirichlet expansion” for the time-evolution function.

Questions concerning the existence and uniqueness of the star exponential as a C^∞ function and the nature of the spectrum and the projectors again require careful mathematical analysis. The problem of finding general conditions on the Hamilton function H which ensure a reasonable physical spectrum is analogous to the problem of showing, in the conventional approach, that the symmetric operator \hat{H} is self-adjoint and finding its spectral projections.

The Simple Harmonic Oscillator

As an example of the above procedure, we treat the simple one-dimensional harmonic oscillator characterized by the classical Hamilton function

$$H(q, p) = \frac{p^2}{2m} + \frac{m\omega^2}{2} q^2 \quad [28]$$

In terms of the holomorphic variables

$$\begin{aligned} a &= \sqrt{\frac{m\omega}{2}} \left(q + i \frac{p}{m\omega} \right), \\ \bar{a} &= \sqrt{\frac{m\omega}{2}} \left(q - i \frac{p}{m\omega} \right) \end{aligned} \quad [29]$$

the Hamilton function becomes

$$H = \omega a \bar{a} \quad [30]$$

Our aim is to calculate the time-evolution function. We first choose a quantization scheme characterized by the normal star product

$$f *_N g = f e^{\hbar \overleftarrow{\partial}_a \overrightarrow{\partial}_{\bar{a}}} g \quad [31]$$

we then have

$$\bar{a} *_N a = a \bar{a}, \quad a *_N \bar{a} = a \bar{a} + \hbar \quad [32]$$

so that

$$[a, \bar{a}]_{*_N} = \hbar \quad [33]$$

Equation [25] for this case is

$$i\hbar \frac{d}{dt} \text{Exp}_N(Ht) = (H + \hbar \omega \bar{a} \partial_{\bar{a}}) \text{Exp}_N(Ht) \quad [34]$$

with the solution

$$\text{Exp}_N(Ht) = e^{-a\bar{a}/\hbar} \exp(e^{-i\omega t} a \bar{a} / \hbar) \quad [35]$$

By expanding the last exponential in eqn [35], we obtain the Fourier–Dirichlet expansion

$$\text{Exp}_N(Ht) = e^{-a\bar{a}/\hbar} \sum_{n=0}^{\infty} \frac{1}{\hbar^n n!} \bar{a}^n a^n e^{-in\omega t} \quad [36]$$

From here, we can read off the energy eigenvalues and the projectors describing the states by comparing coefficients in eqns [27] and [36]:

$$\pi_0^{(N)} = e^{-a\bar{a}/\hbar} \quad [37]$$

$$\pi_n^{(N)} = \frac{1}{\hbar^n n!} \pi_0 \bar{a}^n a^n = \frac{1}{\hbar^n n!} \bar{a}^n *_N \pi_0^{(N)} *_N a^n \quad [38]$$

$$E_n = n\hbar\omega \quad [39]$$

Note that the spectrum obtained in eqn [39] does not include the zero-point energy. The projector onto the ground state $\pi_0^{(N)}$ satisfies

$$a *_N \pi_0^{(N)} = 0 \quad [40]$$

The spectral decomposition of the Hamilton function (eqn [23]) is in this case

$$H = \sum_{n=0}^{\infty} n\hbar\omega \left(\frac{1}{\hbar^n n!} e^{-a\bar{a}/\hbar} \bar{a}^n a^n \right) = \omega a \bar{a} \quad [41]$$

We now consider the Moyal quantization scheme. If we write eqn [12] in terms of holomorphic coordinates, we obtain

$$f *_M g = f \exp\left(\frac{\hbar}{2} (\overleftarrow{\partial}_a \overrightarrow{\partial}_{\bar{a}} - \overleftarrow{\partial}_{\bar{a}} \overrightarrow{\partial}_a)\right) g \quad [42]$$

Here, we have

$$a *_M \bar{a} = a \bar{a} + \frac{\hbar}{2}, \quad \bar{a} *_M a = a \bar{a} - \frac{\hbar}{2} \quad [43]$$

and again

$$[a, \bar{a}]_{*_M} = \hbar \quad [44]$$

The value of the commutator of two phase-space variables is fixed by property (3) of the star product,

and cannot change when one goes to a c -equivalent star product. The Moyal star product is c -equivalent to the normal star product with the transition operator

$$T = e^{-(\hbar/2)\bar{\partial}_a\bar{\partial}_a} \quad [45]$$

We can use this operator to transform the normal product version of the $*$ -genvalue equation, eqn [22], into the corresponding Moyal product version according to eqn [15]. The result is

$$\begin{aligned} H *_M \pi_n^{(M)} &= \omega \left(\bar{a} *_M a + \frac{\hbar}{2} \right) *_M \pi_n^{(M)} \\ &= \hbar\omega \left(n + \frac{1}{2} \right) \pi_n^{(M)} \end{aligned} \quad [46]$$

with

$$\pi_0^{(M)} = T\pi_0^{(N)} = 2e^{-2a\bar{a}/\hbar} \quad [47]$$

$$\pi_n^{(M)} = T\pi_n^{(N)} = \frac{1}{\hbar^n n!} \bar{a}^n *_M \pi_0^{(M)} *_M a^n \quad [48]$$

The projector onto the ground state $\pi_0^{(M)}$ satisfies

$$a *_M \pi_0^{(M)} = 0 \quad [49]$$

We now have, for the spectrum,

$$E_n = \left(n + \frac{1}{2} \right) \hbar\omega \quad [50]$$

which is the textbook result. We conclude that for this problem, the Moyal quantization scheme is the correct one.

The use of the Moyal product in eqn [25] for the star exponential of the harmonic oscillator leads to the following differential equation for the time evolution function:

$$\begin{aligned} i\hbar \frac{d}{dt} \text{Exp}_M(Ht) &= \left(H - \frac{(\hbar\omega)^2}{4} \partial_H - \frac{(\hbar\omega)^2}{4} H \partial_H^2 \right) \text{Exp}_M(Ht) \end{aligned} \quad [51]$$

The solution is

$$\text{Exp}_M(Ht) = \frac{1}{\cos(\omega t/2)} \exp \left[\left(\frac{2H}{i\hbar\omega} \right) \tan \left(\frac{\omega t}{2} \right) \right] \quad [52]$$

This expression can be brought into the form of the Fourier–Dirichlet expansion of eqn [27] by using the generating function for the Laguerre polynomials:

$$\frac{1}{1+s} \exp \left[\frac{zs}{1+s} \right] = \sum_{n=0}^{\infty} s^n (-1)^n L_n(z) \quad [53]$$

with $s = e^{-i\omega t}$. The projectors then become

$$\pi_n^{(M)} = 2(-1)^n e^{-2H/\hbar\omega} L_n \left(\frac{4H}{\hbar\omega} \right) \quad [54]$$

which is equivalent to the expression already found in eqn [48].

Conventional Quantization

One usually finds the observables characterizing some quantum mechanical system by starting from the corresponding classical system, and then, either by guessing or by using some more or less systematic method, and finding the corresponding representations of the classical quantities in the quantum system. The guiding principle is the correspondence principle: the quantum mechanical relations are supposed to reduce somehow to the classical relations in an appropriate limit. Early attempts to systematize this procedure involved finding an assignment rule Θ that associates to each phase-space function f a linear operator in Hilbert space $\hat{f} = \Theta(f)$ in such a way that in the limit $\hbar \rightarrow 0$, the quantum mechanical equations of motion go over to the classical equations. Such an assignment cannot be unique, because even though an operator that is a function of the basic operators \hat{Q} and \hat{P} reduces to a unique phase-space function in the limit $\hbar \rightarrow 0$, there are many ways to assign an operator to a given phase-space function, due to the different orderings of the operators \hat{Q} and \hat{P} that all reduce to the original phase-space function. Different ordering procedures correspond to different quantization schemes. It turns out that there is no quantization scheme for systems with observables that depend on the coordinates or the momenta to a higher power than quadratic which leads to a correspondence between the quantum mechanical and the classical equations of motion, and which simultaneously strictly maintains the Dirac–von Neumann requirement that $(1/i\hbar)[\hat{f}, \hat{g}] \leftrightarrow \{f, g\}$. Only within the framework of deformation quantization does the correspondence principle acquire a precise meaning.

A general scheme for associating phase-space functions and Hilbert space operators, which includes all of the usual orderings, is given as follows: the operator $\Theta_\lambda(f)$ corresponding to a given phase-space function f is

$$\Theta_\lambda(f) = \int \tilde{f}(\xi, \eta) e^{-i(\xi\hat{Q} + \eta\hat{P})} e^{\lambda(\xi, \eta)} d\xi d\eta \quad [55]$$

where \tilde{f} is the Fourier transform of f , and (\hat{Q}, \hat{P}) are the Schrödinger operators that correspond to the phase-space variables (q, p) ; $\lambda(\xi, \eta)$ is a quadratic form:

$$\lambda(\xi, \eta) = \frac{\hbar}{4} (\alpha\eta^2 + \beta\xi^2 + 2i\gamma\xi\eta) \quad [56]$$

Different choices for the constants (α, β, γ) yield different operator ordering schemes.

The relation between operator algebras and star products is given by

$$\Theta(f)\Theta(g) = \Theta(f * g) \quad [57]$$

where Θ is a linear assignment of the kind discussed above. Different assignments, which correspond to different operator orderings, correspond to c -equivalent star products. It demonstrates that the quantum mechanical algebra of observables is a representation of the star product algebra. Because in the algebraic approach to quantum theory all the information concerning the quantum system may be extracted from the algebra of observables, specifying the star product completely determines the quantum system.

The inverse procedure of finding the phase-space function that corresponds to a given operator \hat{f} is, for the special case of Weyl ordering, given by

$$f(q, p) = \int \langle q + \frac{1}{2}\xi | \hat{f} | q - \frac{1}{2}\xi \rangle e^{-i\xi p/\hbar} d\xi \quad [58]$$

When using holonomic coordinates, it is convenient to work with the coherent states

$$\hat{a}|a\rangle = a|a\rangle, \quad \langle \bar{a} | \hat{a}^\dagger = \langle \bar{a} | \bar{a} \quad [59]$$

These states are related to the energy eigenstates of the harmonic oscillator

$$|n\rangle = \frac{1}{\sqrt{n!}} \hat{a}^{\dagger n} |0\rangle \quad [60]$$

by

$$|a\rangle = e^{-\frac{1}{2}\bar{a}\bar{a}/\hbar} \sum_{n=0}^{\infty} \frac{a^n}{\sqrt{n!}} |n\rangle, \quad [61]$$

$$\langle \bar{a} | = e^{-\frac{1}{2}\bar{a}\bar{a}/\hbar} \sum_{n=0}^{\infty} \frac{\bar{a}^n}{\sqrt{n!}} \langle n |$$

In normal ordering, we obtain the phase space function $f(a, \bar{a})$ corresponding to the operator \hat{f} by just taking the matrix element between coherent states:

$$f(a, \bar{a}) = \langle \bar{a} | f(\hat{a}, \hat{a}^\dagger) | a \rangle \quad [62]$$

For holomorphic coordinates, it is easy to show

$$\pi_n^{(N)}(a, \bar{a}) = \frac{1}{\hbar^n} \langle \bar{a} | n \rangle \langle n | a \rangle = \frac{1}{\hbar^n n!} (\bar{a}a)^n e^{-\bar{a}a/\hbar} \quad [63]$$

in agreement with eqn [38] for the normal star product projectors.

The star exponential $\text{Exp}(Ht)$ and the projectors π_n are the phase-space representations of the time-evolution operator $\exp(-i\hat{H}t/\hbar)$ and the projection operators $\hat{\rho}_n = |n\rangle\langle n|$, respectively. Weyl ordering corresponds to the use of the Moyal star product for quantization and normal ordering to the use of the

normal star product. In the density matrix formalism, we say that the projection operator is that of a pure state, which is characterized by the property of being idempotent: $\hat{\rho}_n^2 = \hat{\rho}_n$ (compare eqn [21]). The integral of the projector over the momentum gives the probability distribution in position space:

$$\begin{aligned} \frac{1}{2\pi\hbar} \int \pi_n^{(M)}(q, p) dp \\ = \frac{1}{2\pi\hbar} \int \langle q + \xi/2 | n \rangle \langle n | q - \xi/2 \rangle e^{-i\xi p/\hbar} d\xi dp \\ = \langle q | n \rangle \langle n | q \rangle = |\psi_n(q)|^2 \end{aligned} \quad [64]$$

and the integral over the position gives the probability distribution in momentum space:

$$\frac{1}{2\pi\hbar} \int \pi_n^{(M)}(q, p) dq = \langle p | n \rangle \langle n | p \rangle = |\tilde{\psi}_n(p)|^2 \quad [65]$$

The normalization is

$$\frac{1}{2\pi\hbar} \int \pi_n^{(M)}(q, p) dq dp = 1 \quad [66]$$

which is the same as eqn [20]. Applying these relations to the ground-state projector of the harmonic oscillator, eqn [47] shows that this is a minimum-uncertainty state. In the classical limit $\hbar \rightarrow 0$, it goes to a Dirac δ -function. The expectation value of the Hamiltonian operator is

$$\begin{aligned} \frac{1}{2\pi\hbar} \int (H * \pi_n^{(M)})(q, p) dq dp &= \int \langle q | \hat{H} \hat{\rho}_n | q \rangle dq \\ &= \text{tr}(\hat{H} \hat{\rho}_n) \end{aligned} \quad [67]$$

which should be compared to eqn [24].

Quantum Field Theory

A real scalar field is given in terms of the coefficients $a(\mathbf{k}), \bar{a}(\mathbf{k})$ by

$$\phi(x) = \int \frac{d^3k}{(2\pi)^{3/2} \sqrt{2\omega_k}} \left[a(\mathbf{k}) e^{-ikx} + \bar{a}(\mathbf{k}) e^{ikx} \right] \quad [68]$$

where $\hbar\omega_k = \sqrt{\hbar^2 k^2 + m^2}$ is the energy of a single-quantum of the field. The corresponding quantum field operator is

$$\Phi(x) = \int \frac{d^3k}{(2\pi)^{3/2} \sqrt{2\omega_k}} \left[\hat{a}(\mathbf{k}) e^{-ikx} + \hat{a}^\dagger(\mathbf{k}) e^{ikx} \right] \quad [69]$$

where $\hat{a}(\mathbf{k}), \hat{a}^\dagger(\mathbf{k})$ are the annihilation and creation operators for a quantum of the field with momentum $\hbar\mathbf{k}$. The Hamiltonian is

$$H = \int d^3k \hbar\omega_k \hat{a}^\dagger(\mathbf{k}) \hat{a}(\mathbf{k}) \quad [70]$$

$N(\mathbf{k}) = \hat{a}^\dagger(\mathbf{k})\hat{a}(\mathbf{k})$ is interpreted as the number operator, and eqn [70] is then just the generalization of eqn [39], the expression for the energy of the harmonic oscillator in the normal ordering scheme, for an infinite number of degrees of freedom. Had we chosen the Weyl-ordering scheme, it would have resulted in (by the generalization of eqn [50]) an infinite vacuum energy. Hence, requiring the vacuum energy to vanish implies the choice of the normal ordering scheme in free field theory. In the framework of deformation quantization, this requirement leads to the choice of the normal star product for treating free scalar fields: only for this choice is the star product well defined.

Currently, in realistic physical field theories involving interacting relativistic fields we are limited to perturbative calculations. The objects of interest are products of the fields. The analog of the Moyal product of eqn [11] for systems with an infinite number of degrees of freedom is

$$\begin{aligned} & \phi(x_1) * \phi(x_2) * \cdots * \phi(x_n) \\ &= \exp \left[\frac{1}{2} \sum_{i < j} \int d^4x d^4y \frac{\delta}{\delta \phi_i(x)} \Delta(x-y) \frac{\delta}{\delta \phi_j(y)} \right] \\ & \quad \times \phi_1(x_1), \dots, \phi_n(x_n) \Big|_{\phi_i=\phi} \end{aligned} \quad [71]$$

where the expressions $\delta/\delta\phi(x)$ indicate functional derivatives. Here, we have used the antisymmetric Schwinger function:

$$\Delta(x-y) = [\Phi(x), \Phi(y)] \quad [72]$$

The Schwinger function is uniquely determined by relativistic invariance and causality from the equal-time commutator

$$[\Phi(x), \dot{\Phi}(y)] \Big|_{x^0=y^0} = i\hbar \delta^{(3)}(\mathbf{x}-\mathbf{y}) \quad [73]$$

which is the characterization of the canonical structure in the field theoretic framework.

The Moyal product is, however, not the suitable star product to use in this context. In relativistic quantum field theory, it is necessary to incorporate causality in the form advocated by Feynman: positive frequencies propagate forward in time, whereas negative frequencies propagate backwards in time. This property is achieved by using the Feynman propagator:

$$\Delta_F(x) = \begin{cases} \Delta^+(x) & \text{for } x^0 > 0 \\ -\Delta^-(x) & \text{for } x^0 < 0 \end{cases} \quad [74]$$

where $\Delta^+(x), \Delta^-(x)$ are the propagators for the positive and negative frequency components of the field, respectively. In operator language

$$\Delta_F(x-y) = \mathcal{T}(\Phi(x)\Phi(y)) - \mathcal{N}(\Phi(x)\Phi(y)) \quad [75]$$

where \mathcal{T} indicates the time-ordered product of the fields and \mathcal{N} the normal-ordered product. Because the second term in eqn [75] is a normal-ordered product with vanishing vacuum expectation value, the Feynman propagator may be simply characterized as the vacuum expectation value of the time-ordered product of the fields. The antisymmetric part of the positive frequency propagator is the Schwinger function:

$$\Delta^+(x) - \Delta^+(-x) = \Delta^+(x) + \Delta^-(x) = \Delta(x) \quad [76]$$

The fact that going over to a c -equivalent product leaves the antisymmetric part of the differential operator in the exponent of eqn [71] invariant suggests that the use of the positive frequency propagator instead of the Schwinger function merely involves the passage to a c -equivalent star product. This is indeed easy to verify. The time-ordered product of the operators is obtained by replacing the Schwinger function $\Delta(x-y)$ in eqn [72] by the c -equivalent positive frequency propagator $\Delta^+(x-y)$, restricting the time integration to $x^0 > y^0$, as in eqn [74], and symmetrizing the integral in the variables x and y , which brings in the negative frequency propagator $\Delta^-(x-y)$ for times $x^0 < y^0$. Then eqn [71] becomes Wick's theorem, which is the basic tool of relativistic perturbation theory. In operator language

$$\begin{aligned} & \mathcal{T}(\Phi(x_1), \dots, \Phi(x_n)) \\ &= \exp \left[\frac{1}{2} \int d^4x d^4y \frac{\delta}{\delta \Phi(x)} \Delta_F(x-y) \frac{\delta}{\delta \Phi(y)} \right] \\ & \quad \times \mathcal{N}(\Phi(x_1), \dots, \Phi(x_n)) \end{aligned} \quad [77]$$

Another interesting relation between deformation quantization and quantum field theory has been uncovered by studies of the Poisson-Sigma model. This model involves a set of scalar fields X^i which map a two-dimensional manifold Σ_2 onto a Poisson space M , as well as generalized gauge fields A_i , which are 1-forms on Σ_2 mapping to 1-forms on M . The action is given by

$$S_{PS} = \int_{\Sigma_2} (A_i dX^i + \alpha^{ij} A_i A_j) \quad [78]$$

where α^{ij} is the Poisson structure of M . A remarkable formula was found (Cattaneo and Felder 2000):

$$(f * g)(x) = \int DX D A f(X(1)) g(X(2)) e^{iS_{PS}/\hbar} \quad [79]$$

where f, g are functions on M , $*$ is Kontsevich's star product (Kontsevich 1997), and the functional integration is over all fields X that satisfy the boundary condition $X(\infty) = x$. Here Σ_2 is taken to be a disk in \mathbb{R}^2 ; 1, 2, and ∞ are three points on its circumference. By expanding the functional integral in eqn [79] according to the usual rules of perturbation theory, one finds that the coefficients of the powers of \hbar reproduce the graphs

and weights that characterize Kontsevich's star product. For the case in which the Poisson tensor is invertible, we can perform the Gaussian integration in eqn [79] involving the fields A_i . The result is

$$(f * g)(x) = \int DX f(X(1)) g(X(2)) \exp \left[\frac{i}{\hbar} \int \Omega_{ij} dX^i dX^j \right] \quad [80]$$

Equation [80] is formally similar to eqn [16] for the Moyal product, to which the Kontsevich product reduces in the symplectic case. Here $\Omega_{ij} = (\alpha^{ij})^{-1}$ is the symplectic 2-form, and $\int \Omega_{ij} dX^i dX^j$ is the symplectic volume of the manifold M . To make this relationship exact, one must integrate out the gauge degrees of freedom in the functional integral in eqn [79]. Since the Poisson-sigma model represents a topological field theory there remains only a finite-dimensional integral, which coincides with the integral in eqn [80].

See also: Deformations of the Poisson Bracket on a Symplectic Manifold; Deformation Quantization and Representation Theory; Deformation Theory; Fedosov Quantization; Noncommutative Geometry from Strings; Operads; Quantum Field Theory: A Brief Introduction; Schrödinger Operators.

Further Reading

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Deformation Quantization and Representation Theory

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The Quantization Problem

Though quantum theory for the classical phase space \mathbb{R}^{2n} is well established by means of what usually is called canonical quantization, physics demands to go beyond \mathbb{R}^{2n} : On the one hand, systems with constraints lead by phase-space reduction to classical phase spaces different from \mathbb{R}^{2n} ; in general one ends up with a symplectic or even Poisson manifold. Thus, one needs to quantize geometrically nontrivial phase spaces. On the other hand, field theories and thermodynamical systems require to pass from \mathbb{R}^{2n} to infinitely many degrees of freedom, where one faces additional analytical difficulties. Both types of difficulties combine

for gauge field theories and gravity, whence it is clear that quantization is still one of the most important issues in mathematical physics.

One possibility (among many others) is to use the structural similarity between the classical and quantum observable algebras. In both cases the observables constitute a complex $*$ -algebra: in the classical case it is commutative with the additional structure of a Poisson bracket, whereas in the quantum case the algebra is noncommutative. In deformation quantization, one tries to pass from the classical observables to the quantum observables by a deformation of the algebraic structures.

From Canonical Quantization to Star Products

Let us briefly recall canonical quantization and the ordering problem. In order to “quantize” classical

observables like the polynomials on \mathbb{R}^{2n} to q^k, p_l , one assigns the operators

$$q^k \mapsto \varrho(q^k) = Q^k = (q \mapsto q^k \psi(q)) \quad [1]$$

$$p_l \mapsto \varrho(p_l) = P_l = \left(q \mapsto \frac{\hbar}{i} \frac{\partial \psi}{\partial q^l}(q) \right) \quad [2]$$

for $k, l = 1, \dots, n$, defined on a suitable domain in $L^2(\mathbb{R}^n, d^n q)$. For simplicity, we choose $C_0^\infty(\mathbb{R}^n)$ as domain. The well-known ordering problem is encountered if one wants to also quantize higher polynomials. One convenient (although not the only) possibility is Weyl's total symmetrization rule, that is, for a monomial like $q^2 p$ we take the quantization

$$\begin{aligned} \varrho_{\text{Weyl}}(q^2 p) &= \frac{1}{3} (Q^2 P + Q P Q + P Q^2) \\ &= -i\hbar q^2 \frac{\partial}{\partial q} - i\hbar q \end{aligned} \quad [3]$$

This can be written in the more explicit form:

$$\begin{aligned} \varrho_{\text{Weyl}}(f) &= \sum_{r=0}^{\infty} \frac{1}{r!} \left(\frac{\hbar}{i} \right)^r \frac{\partial^r (Nf)}{\partial p_{i_1} \dots \partial p_{i_r}} \Big|_{p=0} \frac{\partial^r}{\partial q^{i_1} \dots \partial q^{i_r}} \end{aligned} \quad [4]$$

with

$$N = \exp\left(\frac{\hbar}{2i} \Delta\right) \quad \text{and} \quad \Delta = \frac{\partial^2}{\partial q^i \partial p_i}$$

Using [4] one can easily extend ϱ_{Weyl} to all functions $f \in C^\infty(\mathbb{R}^{2n})$ which are polynomial in the momentum variables only and have an arbitrary smooth dependence on the position variables. This Poisson subalgebra of $C^\infty(\mathbb{R}^{2n})$ certainly covers all classical observables of physical interest. Denoting these observables by $\text{Pol}(T^*\mathbb{R}^n)$, one obtains a linear isomorphism

$$\varrho_{\text{Weyl}} : \text{Pol}(T^*\mathbb{R}^n) \xrightarrow{\cong} \text{Diffop}(\mathbb{R}^n) \quad [5]$$

into the differential operators with smooth coefficients, called Weyl symbol calculus. Other orderings would result in a different linear isomorphism like [5], for example, the standard ordering is obtained by simply omitting the operator N in [4].

Using [5], one can pull back the operator product of $\text{Diffop}(\mathbb{R}^n)$ to obtain a new product \star_{Weyl} for $\text{Pol}(T^*\mathbb{R}^n)$, that is

$$f \star_{\text{Weyl}} g = \varrho_{\text{Weyl}}^{-1}(\varrho_{\text{Weyl}}(f) \varrho_{\text{Weyl}}(g)) \quad [6]$$

which is called the Weyl–Moyal star product. Explicitly, one has

$$\begin{aligned} f \star_{\text{Weyl}} g &= \mu \circ \exp\left(\frac{i\hbar}{2} \left(\frac{\partial}{\partial q^k} \otimes \frac{\partial}{\partial p_k} - \frac{\partial}{\partial p_k} \otimes \frac{\partial}{\partial q^k} \right)\right) f \otimes g \end{aligned} \quad [7]$$

where $\mu(f \otimes g) = fg$ is the commutative product. Clearly, for $f, g \in \text{Pol}(T^*\mathbb{R}^n)$ the exponential series terminates after finitely many terms. If one now wants to extend further to all smooth functions, then [7] is only a formal power series in \hbar . Since on a manifold one does not have *a priori* a nice distinguished class of functions like $\text{Pol}(T^*\mathbb{R}^n)$, one indeed has to generalize in this direction if a geometric framework is desired. This observation and the simple fact, that \star_{Weyl} satisfies all the following properties, lead to the definition of a formal star product by Bayen *et al.* (1978):

Definition 1 A formal star product on a Poisson manifold (M, π) is an associative $C[[\lambda]]$ -bilinear product

$$f \star g = \sum_{r=0}^{\infty} \lambda^r C_r(f, g) \quad [8]$$

for $f, g \in C^\infty(M)[[\lambda]]$ such that

1. $C_0(f, g) = fg$ and $C_1(f, g) - C_1(g, f) = i\{f, g\}$,
2. $1 \star f = f = f \star 1$, and
3. C_r is a bidifferential operator.

If in addition $\overline{f \star g} = \bar{g} \star \bar{f}$, then \star is called Hermitian.

Clearly, \star_{Weyl} defines a Hermitian star product for \mathbb{R}^{2n} . The first condition is called the correspondence principle in deformation quantization and the formal parameter $\lambda = \hbar$ corresponds to Planck's constant \hbar once a convergence scheme is established.

If $S = \text{id} + \sum_{r=1}^{\infty} \lambda^r S_r$ is a formal series of differential operators with $S_r 1 = 0$ for $r \geq 1$, then it is easy to see that

$$f \star' g = S^{-1}(Sf \star Sg) \quad [9]$$

defines again a star product which is Hermitian if \star is Hermitian and if in addition $\overline{Sf} = S\bar{f}$. In particular, the operator N , as before, serves for the transition from \star_{Weyl} to the standard-ordered star product \star_{Std} obtained the same way from the standard-ordered quantization. Thus, [9] can be seen as the abstract notion of changing the ordering prescription, even if no operator representation has been specified. Two star products related by such an equivalence transformation are called equivalent and \ast -equivalent in the Hermitian case.

One main advantage of formal deformation quantization is that one has very strong existence and classification results:

Theorem 2 On every Poisson manifold there exists a star product.

The above theorem was first shown by deWilde and Lecomte (1983) for the symplectic case and

independently by Fedosov (1985) and Omori, Maeda, and Yoshioka (1991). In 1997, Kontsevich was able to prove the general Poisson case by showing his profound formality theorem. The full classification of star products up to equivalence was first obtained for the symplectic case by Nest and Tsygan (1995) and independently by Deligne (1995), Bertelson, Cahen, and Gutt (1997), and Weinstein and Xu (1997). The general Poisson case again follows from Kontsevich's formality. In particular, in the symplectic case, star products are classified by their characteristic class

$$c : \star \mapsto c(\star) \in \frac{[\omega]}{i\lambda} + H_{\text{deRham}}^2(M, \mathbb{C})[[\lambda]] \quad [10]$$

As conclusion one can state that for the price of formal power series in \hbar one obtains in formal deformation quantization a very general and well-understood picture of the observable algebra for the quantum version of any classical system described kinematically by a Poisson manifold. It turns out that already in this framework one can discuss dynamics as well by use of a Heisenberg equation formulated with \star . Moreover, the quantization of symmetries described by Hamiltonian Lie group or Lie algebra actions has been extensively studied.

For a physical theory of quantization, however, there are still at least two ingredients missing. On the one hand, one has to overcome the formal power series expansion in \hbar . This problem is, in principle, on the same footing as any perturbative approach to quantum theory and thus no easy answer can be expected to hold in general. In particular examples, however, such as the Weyl-Moyal star product, it can easily be solved. These issues together with the corresponding questions about a spectral calculus are best studied in the framework of Rieffel's strict deformation quantization based on a more C^* -algebraic formulation of the deformation problem. On the other hand, the observable algebra is not enough to describe a quantum system: one also needs to have a notion for the states. It turns out that already in the formal framework one has a physically reasonable notion of states as discussed by Bordemann and Waldmann (1998).

States and Representations

The notion of states in deformation quantization is adapted from the C^* -algebraic world and based on the notion of positive functionals. Recall that for a \star -algebra \mathcal{A} over \mathbb{C} a linear functional

$\omega : \mathcal{A} \rightarrow \mathbb{C}$ is called positive if $\omega(a^*a) \geq 0$. For formal deformation quantization, things are slightly more subtle as now one has to consider $\mathbb{C}[[\lambda]]$ -linear functionals

$$\omega : (C^\infty(M)[[\lambda]], \star) \longrightarrow \mathbb{C}[[\lambda]] \quad [11]$$

where \star is assumed to be a Hermitian star product in the following. Then the positivity is understood in the sense of formal power series where $a \in \mathbb{R}[[\lambda]]$ is called positive if $a = \sum_{r=0}^{\infty} \lambda^r a_r$ with $a_{r_0} > 0$. Thus, we can make sense out of the following requirement:

Definition 3 Let \star be a Hermitian star product on M . A $\mathbb{C}[[\lambda]]$ -linear functional $\omega : C^\infty(M)[[\lambda]] \rightarrow \mathbb{C}[[\lambda]]$ is called positive with respect to \star if

$$\omega(\bar{f} \star f) \geq 0 \quad [12]$$

and it is called a state if, in addition, $\omega(1) = 1$.

In fact, $\omega(f)$ is interpreted as the expectation value of the observable f in the state ω . The positivity [12] ensures that the usual uncertainty relations between expectation values hold.

Sometimes it is convenient to consider positive functionals only defined on a (proper) \star -ideal in $C^\infty(M)[[\lambda]]$, for instance, $C_0^\infty(M)[[\lambda]]$.

Since in some situations one wants more general formal series than just power series, it is convenient to embed the above definition of states into a larger and more algebraic context: consider an ordered ring R , that is, a commutative, associative, unital ring R together with a distinguished subset $P \subset R$ (the positive elements) such that R is the disjoint union $-P \dot{\cup} \{0\} \dot{\cup} P$, and we have $P \cdot P \subseteq P$ and $P + P \subseteq P$. Then $\mathbb{C} = R(i)$ denotes the ring extension by a square root i of -1 and consider \star -algebras \mathcal{A} over \mathbb{C} . Clearly, this generalizes the cases $R = \mathbb{R}$, where $\mathbb{C} = \mathbb{C}$, as well as $R = \mathbb{R}[[\lambda]]$, where $\mathbb{C} = \mathbb{C}[[\lambda]]$. In this way, one provides a framework where C^* -algebras, \star -algebras over \mathbb{C} , and formal Hermitian star products can be treated on the same footing. It is clear that the definition of a positive functional immediately extends to $\omega : \mathcal{A} \rightarrow \mathbb{C}$ for such a ring \mathbb{C} .

Example 4

- (i) For the Wick star product on $\mathbb{R}^{2n} \cong \mathbb{C}^n$, defined by

$$f \star_{\text{Wick}} g = \sum_{r=0}^{\infty} \frac{(2\lambda)^r}{r!} \frac{\partial^r f}{\partial z^{i_1} \dots \partial z^{i_r}} \frac{\partial^r g}{\partial \bar{z}^{i_1} \dots \partial \bar{z}^{i_r}} \quad [13]$$

the δ -functional $\delta : f \mapsto f(0)$ is positive. Note, however, that δ is not positive for \star_{Weyl} .

- (ii) For the Weyl–Moyal star product \star_{Weyl} the Schrödinger functional

$$\omega(f) = \int_{\mathbb{R}^n} f(q, p=0) d^n q \quad [14]$$

defined on the \ast -ideal $C_0^\infty(\mathbb{R}^{2n})[[\lambda]]$, is positive.

- (iii) For any connected symplectic manifold (M, ω) and any Hermitian star product \star , there exists a unique normalized trace functional

$$\begin{aligned} \text{tr} : C_0^\infty(M)[[\lambda]] &\longrightarrow \mathbb{C}[[\lambda]] \\ \text{tr}(f \star g) &= \text{tr}(g \star f) \end{aligned} \quad [15]$$

with zeroth order equal to the integration over M with respect to the Liouville measure $\Omega = \omega^n$. Then this trace is positive as well, $\text{tr}(\bar{f} \star f) \geq 0$.

Having a notion for states as expectation-value functionals is still not enough to formulate quantum theory. One main feature of quantum states, the superposition principle, is not yet implemented. In particular, forming convex combinations like $\omega = c_1 \omega_1 + c_2 \omega_2$, with $c_1, c_2 \geq 0$ and $c_1 + c_2 = 1$, does not give a superposition of ω_1 and ω_2 but a mixed state. Hence, one needs an additional linear structure on the states whence we look for a \ast -representation π of the observable algebra \mathcal{A} on a pre-Hilbert space \mathcal{H} over \mathbb{C} such that the states ω_1, ω_2 can be written as vector states $\omega_i(a) = \langle \phi_i, \pi(a) \phi_i \rangle$ for some unit vectors $\phi_1, \phi_2 \in \mathcal{H}$. Then one can build superpositions of the vectors ϕ_1, ϕ_2 in the usual way. While this is the well-known argument in any quantum theory based on the observable algebras, for deformation quantization one first has to make sense out of the above notions, since now $\mathbb{R} = \mathbb{R}[[\lambda]]$ is only an ordered ring. This can actually be done in a consistent way as demonstrated and exemplified by Bordemann, Bursztyn, Waldmann, and others.

We recall the basic results: A pre-Hilbert space \mathcal{H} over \mathbb{C} is a \mathbb{C} -module with a \mathbb{C} -sesquilinear inner product $\langle \cdot, \cdot \rangle : \mathcal{H} \times \mathcal{H} \rightarrow \mathbb{C}$ such that $\langle \phi, \psi \rangle = \overline{\langle \psi, \phi \rangle}$ and $\langle \phi, \phi \rangle > 0$ for $\phi \neq 0$. This makes sense since \mathbb{R} is ordered. An operator $A : \mathcal{H}_1 \rightarrow \mathcal{H}_2$ is called adjointable if there exists an operator $A^* : \mathcal{H}_2 \rightarrow \mathcal{H}_1$ such that $\langle A\phi, \psi \rangle_2 = \langle \phi, A^*\psi \rangle_1$ for all $\phi \in \mathcal{H}_1, \psi \in \mathcal{H}_2$. The set of adjointable operators is denoted by $\mathfrak{B}(\mathcal{H}_1, \mathcal{H}_2)$, and $\mathfrak{B}(\mathcal{H}) = \mathfrak{B}(\mathcal{H}, \mathcal{H})$ turns out to be a \ast -algebra over \mathbb{C} . This allows one to define a \ast -representation π of \mathcal{A} on \mathcal{H} to be a \ast -homomorphism $\pi : \mathcal{A} \rightarrow \mathfrak{B}(\mathcal{H})$. An intertwiner T between two \ast -representations (\mathcal{H}_1, π_1) and (\mathcal{H}_2, π_2) is an operator $T \in \mathfrak{B}(\mathcal{H}_1, \mathcal{H}_2)$ with $T\pi_1(a) = \pi_2(a)T$ for all $a \in \mathcal{A}$. This defines the category $\ast\text{-Rep}(\mathcal{A})$ of \ast -representations of \mathcal{A} .

Let us now recall that a positive linear functional ω can be written as an expectation value for a vector

state in some representation. This is the well-known Gelfand–Naimark–Segal (GNS) construction from operator algebra theory which can be transferred to this purely algebraic context (Bordemann and Waldmann 1998). First recall that any positive linear functional $\omega : \mathcal{A} \rightarrow \mathbb{C}$ satisfies the Cauchy–Schwarz inequality

$$\omega(a^*b)\overline{\omega(a^*b)} \leq \omega(a^*a)\omega(b^*b) \quad [16]$$

and $\omega(a^*b) = \overline{\omega(b^*a)}$. If \mathcal{A} is unital, which will always be assumed for simplicity, then $\omega(a^*) = \overline{\omega(a)}$ follows. Then

$$\mathcal{I}_\omega = \{a \in \mathcal{A} \mid \omega(a^*a) = 0\} \quad [17]$$

is a left ideal in \mathcal{A} , the so-called Gel'fand ideal, and hence $\mathcal{H}_\omega = \mathcal{A}/\mathcal{I}_\omega$ is a left \mathcal{A} -module with module structure denoted by $\pi_\omega(a)\psi_b = \psi_{ab}$, where $\psi_b \in \mathcal{H}_\omega$ denotes the equivalence class of $b \in \mathcal{A}$. Finally, $\langle \psi_b, \psi_c \rangle = \omega(b^*c)$ turns \mathcal{H}_ω into a pre-Hilbert space and π_ω becomes a \ast -representation, the GNS representation with respect to ω . Moreover, $\psi_1 \in \mathcal{H}_\omega$ is a cyclic vector, $\psi_b = \pi_\omega(b)\psi_1$, with the property

$$\omega(a) = \langle \psi_1, \pi_\omega(a)\psi_1 \rangle \quad [18]$$

These properties characterize the GNS representation $(\mathcal{H}_\omega, \pi_\omega, \psi_1)$ up to unitary equivalence.

Example 5 We can now apply this construction to the three basic examples and obtain the following well-known representations as GNS representations:

- (i) The GNS representation corresponding to the δ -functional and the Wick star product is (unitarily equivalent to) the formal Bargmann–Fock representation. Here $\mathcal{H}_\delta = \mathbb{C}[[\bar{y}^1, \dots, \bar{y}^n]][[\lambda]]$ with inner product

$$\begin{aligned} \langle \phi, \psi \rangle &= \sum_{r=0}^{\infty} \frac{(2\lambda)^r}{r!} \frac{\partial^r \phi}{\partial \bar{y}^{i_1} \dots \partial \bar{y}^{i_r}}(0) \\ &\quad \times \frac{\partial^r \psi}{\partial \bar{y}^{j_1} \dots \partial \bar{y}^{j_r}}(0) \end{aligned} \quad [19]$$

and π_δ is explicitly given by

$$\begin{aligned} \pi_\delta(f) &= \sum_{r,s=0}^{\infty} \frac{(2\lambda)^r}{r!s!} \frac{\partial^{r+s} f}{\partial z^{i_1} \dots \partial z^{i_r} \partial \bar{z}^{j_1} \dots \partial \bar{z}^{j_s}}(0) \\ &\quad \times \bar{y}^{j_1} \dots \bar{y}^{j_s} \frac{\partial^r}{\partial \bar{y}^{i_1} \dots \partial \bar{y}^{i_r}} \end{aligned} \quad [20]$$

In particular, $\pi_\delta(z^j) = 2\lambda \partial / \partial \bar{y}^j$ and $\pi_\delta(\bar{z}^j) = \bar{y}^j$ are the annihilation and creation operators and [20] gives the Wick (or normal) ordering. This basic example has been extended to arbitrary Kähler manifolds by Bordemann and Waldmann (1998).

- (ii) The Weyl–Moyal star product \star_{Weyl} and the Schrödinger functional ω as in [14] give the usual Schrödinger representation as GNS representation. We obtain $\mathcal{H}_\omega = C_0^\infty(\mathbb{R}^n)[[\lambda]]$ with inner product

$$\langle \phi, \psi \rangle = \int_{\mathbb{R}^n} \overline{\phi(q)} \psi(q) d^n q \quad [21]$$

and $\pi_\omega(f) = \varrho_{\text{Weyl}}(f)$ as in [4] with \hbar replaced by λ . The Schrödinger representation as a particular case of a GNS representation has been generalized to arbitrary cotangent bundles including representations on sections of line bundles over the configuration space (Dirac's representation for magnetic monopoles) by Bordemann, Neumaier, Pflaum, and Waldmann (1999, 2003). In this context, the WKB expansion can also be formulated.

- (iii) For the positive trace tr , the GNS pre-Hilbert is simply the space $\mathcal{H}_{\text{tr}} = C_0^\infty(M)[[\lambda]]$ with inner product $\langle f, g \rangle = \text{tr}(\bar{f} \star g)$. The corresponding GNS representation is the left regular representation $\pi_{\text{tr}}(f)g = f \star g$. Note that in this case the commutant of the representation is (anti-)isomorphic to the observable algebra and given by all the right multiplications. Thus, π_{tr} is highly reducible and the size of the commutant indicates a “thermodynamical” interpretation of this representation. Indeed, one can take this GNS representation, and more general for arbitrary KMS functionals, as a starting point of a preliminary version of a Tomita–Takesaki theory for deformation quantization as shown by Waldmann (1999).

After these fundamental examples, we now reconsider the question of superpositions: in general, two (pure) states ω_1, ω_2 cannot be realized as vector states inside a single irreducible representation. One encounters superselection rules. Usually, for instance, in algebraic quantum field theory, the existence of superselection rules indicates the presence of charges. In particular, it is not sufficient to consider one single representation of the observable algebra \mathcal{A} . Instead, one has to investigate (as good as possible) all superselection sectors of the representation theory $\ast\text{-Rep}(\mathcal{A})$ of \mathcal{A} and find physically motivated criteria to select distinguished representations. In usual quantum mechanics on \mathbb{R}^{2n} , this turns out to be rather simple, thanks to the (nontrivial) uniqueness theorem of von Neumann: one has a unique irreducible representation of the Weyl algebra up to unitary equivalence. In infinite dimensions or in topologically nontrivial situations, however, von Neumann's theorem does not apply and one indeed has superselection rules.

In deformation quantization, some parts of these superselection rules have been understood well: again, for cotangent bundles T^*Q , one can classify the unitary equivalence classes of Schrödinger-like representations on $C_0^\infty(Q)[[\lambda]]$ by topological classes of nontrivial vector potentials. Thus, one arrives at the interpretation of the Aharonov–Bohm effect as superselection rule where the classification is essentially given by $H_{\text{deRham}}^1(Q, \mathbb{C})/2\pi i H_{\text{deRham}}^1(Q, \mathbb{Z})$.

General Representation Theory

Although it is very much desirable to determine the structure and the superselection sectors in $\ast\text{-Rep}(\mathcal{A})$ completely, this is only achievable in the very simplest examples. Moreover, for formal star products, many artifacts due to the purely algebraic nature have to be expected: the Bargmann–Fock and Schrödinger representation in Example 5 are unitarily inequivalent and thus define a superselection rule, even the pre-Hilbert spaces are nonisomorphic. However, these artifacts vanish immediately when one imposes the suitable convergence conditions together with appropriate topological completions (von Neumann's theorem). Given such problems, it is very difficult to find “hard” superselection rules which indeed have physical significance already at the formal level. Nevertheless, the example of the Aharonov–Bohm effect shows that this is possible. In any case, new techniques for investigating $\ast\text{-Rep}(\mathcal{A})$ have to be developed. It turns out that comparing $\ast\text{-Rep}(\mathcal{A})$ with some other $\ast\text{-Rep}(\mathcal{B})$ is much simpler but still gives some nontrivial insight in the structure of the representation theory. Here the Morita theory provides a highly sophisticated tool.

The classical notion of Morita equivalence as well as Rieffel's more specialized strong Morita equivalence for C^* -algebras have been transferred to deformation quantization and, more generally, to \ast -algebras \mathcal{A} over $\mathbb{C} = \mathbb{R}(i)$ by Bursztyn and Waldmann (2001). The aim is to construct functors

$$F : \ast\text{-Rep}(\mathcal{A}) \longrightarrow \ast\text{-Rep}(\mathcal{B}) \quad [22]$$

which allow us to compare these categories and determine whether they are equivalent. But even if they are not equivalent, functors such as [22] are interesting. As example, one considers the situation of classical phase space reduction $M \leadsto M_{\text{red}}$ as it is present in every constraint system or gauge theory. Suppose one succeeded with the (highly nontrivial) problem of quantizing both classical phase spaces in a reasonable way whence one has quantum observable algebras \mathcal{A} and \mathcal{A}_{red} . Then, of course, a relation between $\ast\text{-Rep}(\mathcal{A})$ and $\ast\text{-Rep}(\mathcal{A}_{\text{red}})$ is of

particular physical interest although one cannot expect both representation theories to be equivalent: \mathcal{A} contains additional but physically irrelevant structure leading to possibly “more” representations.

To get a clear picture of the Morita theory, one has to extend the notion of $*$ -representations to the following framework: for an auxiliary $*$ -algebra \mathcal{D} over \mathbb{C} , one defines a pre-Hilbert right \mathcal{D} -module to be a right \mathcal{D} -module \mathcal{H} together with a \mathbb{C} -sesquilinear \mathcal{D} -valued inner product $\langle \cdot, \cdot \rangle : \mathcal{H} \times \mathcal{H} \rightarrow \mathcal{D}$ such that $\langle \phi, \psi \rangle^*$ and $\langle \phi, \psi \cdot d \rangle = \langle \phi, \psi \rangle d$ for $d \in \mathcal{D}$ and such that $\langle \cdot, \cdot \rangle$ is completely positive. This means $(\langle \phi_i, \phi_j \rangle) \in M_n(\mathcal{D})^+$ for all ϕ_1, \dots, ϕ_n , where, in general, an algebra element $a \in \mathcal{A}$ is called positive, $a \in \mathcal{A}^+$, if $\omega(a) \geq 0$ for all positive linear functionals $\omega : \mathcal{A} \rightarrow \mathbb{C}$.

Then one defines $\mathfrak{B}(\mathcal{H})$ analogously as for pre-Hilbert spaces leading to a definition of a $*$ -representation π of \mathcal{A} on a pre-Hilbert right \mathcal{D} -module \mathcal{H} . The corresponding category of $*$ -representations is denoted by $*\text{-Rep}_{\mathcal{D}}(\mathcal{A})$. Clearly, elements in $*\text{-Rep}_{\mathcal{D}}(\mathcal{A})$ are in particular $(\mathcal{A}, \mathcal{D})$ -bimodules.

The advantage is that now one has a tensor product $\hat{\otimes}$ taking care of the inner products as well. For $*$ -algebras $\mathcal{A}, \mathcal{B}, \mathcal{C}$, one has a functor

$$\hat{\otimes} : *\text{-Rep}_{\mathcal{B}}(\mathcal{C}) \times *\text{-Rep}_{\mathcal{A}}(\mathcal{B}) \longrightarrow *\text{-Rep}_{\mathcal{A}}(\mathcal{C}) \quad [23]$$

which, on objects, is essentially given by $\otimes_{\mathcal{B}}$. In fact, for $\mathcal{F} \in *\text{-Rep}_{\mathcal{B}}(\mathcal{C})$ and $\mathcal{E} \in *\text{-Rep}_{\mathcal{A}}(\mathcal{B})$, one defines on the $(\mathcal{C}, \mathcal{A})$ -bimodule $\mathcal{F} \otimes_{\mathcal{B}} \mathcal{E}$ an \mathcal{A} -valued inner product by $\langle x \otimes \phi, y \otimes \psi \rangle = \langle \phi, \langle x, y \rangle \cdot \psi \rangle$, which turns out to be well defined and completely positive again. Then $\mathcal{F} \hat{\otimes} \mathcal{E}$ is $\mathcal{F} \otimes_{\mathcal{B}} \mathcal{E}$ equipped with this inner product modulo its possibly nonempty degeneracy space.

By fixing one of the arguments of $\hat{\otimes}$, one obtains the functor of Rieffel induction of $*$ -representations

$$R_{\mathcal{E}} : *\text{-Rep}_{\mathcal{D}}(\mathcal{A}) \longrightarrow *\text{-Rep}_{\mathcal{D}}(\mathcal{B}) \quad [24]$$

where $\mathcal{E} \in *\text{-Rep}_{\mathcal{A}}(\mathcal{B})$ is fixed and $R_{\mathcal{E}}(\mathcal{H}) = \mathcal{E} \hat{\otimes} \mathcal{H}$ for $\mathcal{H} \in *\text{-Rep}_{\mathcal{D}}(\mathcal{A})$.

The idea of strong Morita equivalence is then to search for such bimodules \mathcal{E} where $R_{\mathcal{E}}$ gives an equivalence of categories. In detail, this is accomplished by the following definition, where, for simplicity, only unital $*$ -algebras are considered.

Definition 6 A $(\mathcal{B}, \mathcal{A})$ -bimodule \mathcal{E} is called a strong Morita equivalence bimodule if it is equipped with completely positive inner products $\langle \cdot, \cdot \rangle_{\mathcal{A}}$ and $\langle \cdot, \cdot \rangle_{\mathcal{B}}$ such that both inner products are full, in the sense that

$$\mathbb{C}\text{-span}\{\langle x, y \rangle_{\mathcal{A}} | x, y \in \mathcal{E}\} = \mathcal{A} \quad [25]$$

and analogously for $\langle \cdot, \cdot \rangle_{\mathcal{B}}$, and compatible, in the sense that

$$\langle b \cdot x, y \rangle_{\mathcal{A}} = \langle x, b^* \cdot y \rangle_{\mathcal{A}}, \quad \langle x \cdot a, y \rangle_{\mathcal{B}} = \langle x, y \cdot a^* \rangle_{\mathcal{B}} \quad [26]$$

$$\langle x, y \rangle_{\mathcal{B}} \cdot z = x \cdot \langle y, z \rangle_{\mathcal{A}} \quad [27]$$

In this case, \mathcal{A} and \mathcal{B} are called strongly Morita equivalent.

It turns out that this is indeed an equivalence relation and that strong Morita equivalence implies the equivalence of the representation theories:

Theorem 7 For unital $*$ -algebras over \mathbb{C} , strong Morita equivalence is an equivalence relation.

Theorem 8 If \mathcal{E} is a strong Morita equivalence bimodule, then $R_{\mathcal{E}}$ as in [24] is an equivalence of categories.

Example 9 The fundamental example in Morita theory is that a unital $*$ -algebra \mathcal{A} is strongly Morita equivalent to the matrices $M_n(\mathcal{A})$ via the $(M_n(\mathcal{A}), \mathcal{A})$ -bimodule \mathcal{A}^n where the inner product is $\langle x, y \rangle_{\mathcal{A}} = \sum_{i=1}^n x_i^* y_i$ and $\langle \cdot, \cdot \rangle_{M_n(\mathcal{A})}$ is uniquely determined by the compatibility condition [27].

An efficient way to encode the whole Morita theory of unital $*$ -algebras over \mathbb{C} is to collect all strong Morita equivalence bimodules modulo isometric isomorphisms of bimodules. Then the tensor product $\hat{\otimes}$ makes this into a “large” groupoid whose units are the $*$ -algebras themselves. This so-called Picard groupoid Pic then encodes everything one can say about strong Morita equivalence. In particular, the orbits of this groupoid are precisely the strong Morita equivalence classes of $*$ -algebras. The isotropy groups are the Picard groups $\text{Pic}(\mathcal{A})$ which generalize the (outer) automorphism groups.

Strong Morita Equivalence of Star Products

This section considers star products from the viewpoint of the Morita equivalence. Here one can show that for $\mathcal{A} = (C^\infty(M)[[\lambda]], \star)$, the possible candidates of equivalence bimodules are formal power series of sections $\Gamma^\infty(E)[[\lambda]]$ of vector bundles $E \rightarrow M$. This follows as, on the one hand, strong Morita equivalence is compatible with the classical limit $\lambda=0$ in the sense that it implies strong Morita equivalence of the classical limits. On the other hand, any (classical or quantum) equivalence bimodule is finitely generated and projective as right \mathcal{A} -module. Thus, by the Serre–Swan theorem one obtains the sections of a vector bundle in the

classical limit. Now one can show that every vector bundle can uniquely (up to equivalence) be deformed such that $\Gamma^\infty(E)[[\lambda]]$ becomes a right \mathcal{A} -module. Thus, the only thing to be computed is which deformation \star' is induced by this deformation of E for the endomorphisms $\Gamma^\infty(\text{End}(E))[[\lambda]]$, since one can show that then the result will always be a strong Morita equivalence bimodule. The inner products come from deformations of a Hermitian fiber metric on E .

Since every vector bundle $E \rightarrow M$ can be deformed in this manner in an essentially unique way, we arrive at a general global construction of a noncommutative field theory where the fields are sections of E endowed with a deformed bimodule structure. In the case where M is even a symplectic manifold, a simple extension of Fedosov's construction of a star product \star gives a rather explicit formula for the deformed bimodule structure of $\Gamma^\infty(E)[[\lambda]]$ including a construction of the deformation $(\Gamma^\infty(\text{End}(E))[[\lambda]], \star')$ which acts from the left. As usual in Fedosov's approach, the construction depends functorially on the choice of a connection ∇^E for E .

Returning to the question of strong Morita equivalence of star products, we see that the vector bundle E has to be a line bundle L since only in this case we have $\Gamma^\infty(\text{End}(E)) \cong C^\infty(M)$. Since the deformation of the Hermitian fiber metric is always possible and since two equivalent Hermitian star products are always \ast -equivalent, one can show that strong Morita equivalence is already implied by ring-theoretic Morita equivalence (the converse is true in general).

Theorem 10 *Star products are strongly Morita equivalent if and only if they are Morita equivalent.*

An analogous statement holds for C^* -algebras, known as Beer's theorem (1982).

In the symplectic case, the characteristic class $c(\star')$ of the induced star product \star' can be computed explicitly leading to the following classification by Bursztyn and Waldmann (2002):

Theorem 11 *Let \star, \star' be star products on a symplectic manifold M . Then \star' is (strongly) Morita equivalent to \star if and only if there exists a symplectomorphism ψ such that*

$$\psi^* c(\star') - c(\star) \in 2\pi i H_{\text{deRham}}^2(M, \mathbb{Z}) \quad [28]$$

A similar result in the general Poisson case was given by Jurčo, Schupp, and Wess (2002) based on Kontsevich's formality theorem. This approach is motivated by a careful investigation of noncommutative (scalar) field theories.

Finally, it is worth mentioning that [28] has a very simple physical interpretation. Consider again a cotangent bundle T^*Q with a topologically non-trivial configuration space Q , for example, $\mathbb{R}^3 \setminus \{0\}$. Then there is a canonical Weyl-type star product \star_{Weyl} depending on the choice of a connection ∇ and an integration density $\mu > 0$, generalizing [7] to a curved situation. Now let B be a magnetic field, modeled as a closed 2-form on Q . Minimal coupling leads to a new star product \star_{Weyl}^B describing an electrically charged particle moving in Q in the external field B . Then the two star products \star_{Weyl} and \star_{Weyl}^B are (strongly) Morita equivalent if and only if the magnetic field satisfies Dirac's integrality condition for the (possibly nontrivial) magnetic charges described by B . Thus, Dirac's condition is responsible for the very strong statement that the quantizations with and without magnetic field are Morita equivalent. In particular, the \ast -representation theories of \star_{Weyl} and \star_{Weyl}^B are equivalent. Even more specifically, using B to construct a line bundle $L \rightarrow Q$ one obtains the result that Dirac's \ast -representation of \star_{Weyl}^B on $\Gamma_0^\infty(L)[[\lambda]]$ is precisely the Rieffel induction of the Schrödinger representation of \star_{Weyl} on $C_0^\infty(Q)[[\lambda]]$.

See also: Aharonov–Bohm Effect; Algebraic Approach to Quantum Field Theory; Deformation Quantization; Deformation Theory; Deformations of the Poisson Bracket on a Symplectic Manifold; Fedosov Quantization.

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Deformation Theory

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Introduction and Historical Remarks

In mathematical deformation theory one studies how an object in a certain category of spaces can be varied as a function of the points of a parameter space. In other words, deformation theory thus deals with the structure of families of objects like varieties, singularities, vector bundles, coherent sheaves, algebras, or differentiable maps. Deformation problems appear in various areas of mathematics, in particular in algebra, algebraic and analytic geometry, and mathematical physics. According to Deligne, there is a common philosophy behind all deformation problems in characteristic zero. It is the goal of this survey to explain this point of view. Moreover, we will provide several examples with relevance for mathematical physics.

Historically, modern deformation theory has its roots in the work of Grothendieck, Artin, Quillen, Schlessinger, Kodaira–Spencer, Kuranishi, Deligne, Grauert, Gerstenhaber, and Arnol'd. The application of deformation methods to quantization theory goes back to Bayen–Flato–Fronsdal–Lichnerowicz–Sternheimer, and has led to the concept of a star product on symplectic and Poisson manifolds. The existence of such star products has been proved by de Wilde–Lecomte

and Fedosov for symplectic and by Kontsevich for Poisson manifolds.

Recently, Fukaya and Kontsevich have found a far-reaching connection between general deformation theory, the theory of moduli, and mirror symmetry. Thus, deformation theory comes back to its origins, which lie in the desire to construct moduli spaces. Briefly, a moduli problem can be described as the attempt to collect all isomorphism classes of spaces of a certain type into one single object, the moduli space, and then to study its geometric and analytic properties. The observations by Fukaya and Kontsevich have led to new insight into the algebraic geometry of mirror varieties and their application to string theory.

Basic Definitions and Examples

Deformation theory is based on the notion of a ringed space, so we briefly recall its definition.

Definition 1 Let k be a field. By a k -ringed space one understands a topological space X together with a sheaf \mathcal{A} of unital k -algebras on X . The sheaf \mathcal{A} will be called the structure sheaf of the ringed space. In case each of the stalks $\mathcal{A}_x, x \in X$, is a local algebra, that is, has a unique maximal ideal \mathfrak{m}_x , one calls (X, \mathcal{A}) a locally k -ringed space. Likewise, one defines a commutative k -ringed space as a ringed space such that the stalks of the structure sheaf are all commutative.

Given two k -ringed spaces (X, \mathcal{A}) and (Y, \mathcal{B}) , a morphism from (X, \mathcal{A}) to (Y, \mathcal{B}) is a pair (f, φ) , where

$f: X \rightarrow Y$ is a continuous mapping and $\varphi: f^{-1}\mathcal{B} \rightarrow \mathcal{A}$ a morphism of sheaves of algebras. This means in particular that for every point $x \in X$ there is a homomorphism of algebras $\varphi_x: \mathcal{B}_{f(x)} \rightarrow \mathcal{A}_x$ induced by φ . Under the assumption that both ringed spaces are local, (f, φ) is called a morphism of locally ringed spaces, if each φ_x is a homomorphism of local \mathbb{k} -algebras, that is, maps the maximal ideal of $\mathcal{B}_{f(x)}$ to the one of \mathcal{A}_x .

Clearly, \mathbb{k} -ringed spaces (resp. locally or commutative \mathbb{k} -ringed spaces) together with their morphisms form a category. The following is a list of examples of ringed spaces, in particular of those which will be needed later.

Example 2

- (i) Denote by \mathcal{C}^∞ the sheaf of smooth functions on \mathbb{R}^n , by \mathcal{C}^ω the sheaf of real analytic functions, and let \mathcal{O} be the sheaf of holomorphic functions on \mathbb{C}^n . Then $(\mathbb{R}^n, \mathcal{C}^\infty)$, $(\mathbb{R}^n, \mathcal{C}^\omega)$, and $(\mathbb{C}^n, \mathcal{O})$ are ringed spaces over \mathbb{R} resp. \mathbb{C} .
- (ii) A differentiable manifold of dimension n can be understood as a locally \mathbb{R} -ringed space $(M, \mathcal{C}_M^\infty)$ which locally is isomorphic to $(\mathbb{R}^n, \mathcal{C}^\infty)$. Likewise, a real analytic manifold is a ringed space $(M, \mathcal{C}_M^\omega)$ which locally can be modeled by $(\mathbb{R}^n, \mathcal{C}^\omega)$, and a complex manifold is an (M, \mathcal{O}_M) which locally looks like $(\mathbb{C}^n, \mathcal{O})$.
- (iii) Let D be a domain in \mathbb{C}^n , and \mathcal{I} an ideal sheaf in \mathcal{O}_D of finite type, which means that \mathcal{I} is locally finitely generated over \mathcal{O}_D . Let Y be the support of the quotient sheaf $\mathcal{O}_D/\mathcal{I}$. The pair (Y, \mathcal{O}_Y) , where \mathcal{O}_Y denotes the restriction of $\mathcal{O}_D/\mathcal{I}$ to Y , then is a ringed space, called a complex model space. A complex space now is a ringed space (X, \mathcal{O}_X) which locally looks like a complex model space (cf. Grauert and Remmert 1984).
- (iv) Let \mathbb{k} be an algebraically closed field, and \mathbb{A}^n the affine space over \mathbb{k} of dimension n . Then \mathbb{A}^n , together with the sheaf of regular functions, is a ringed space.
- (v) Given a ring A , its spectrum $\text{Spec } A$ together with the sheaf of regular functions \mathcal{O}_A forms a ringed space (cf. (Hartshorne (1997), section II.2)). One calls $(\text{Spec } A, \mathcal{O}_A)$ an affine scheme. More generally, a scheme is a ringed space (X, \mathcal{O}_X) which locally can be modeled by affine schemes.
- (vi) Finally, if A is a local \mathbb{k} -algebra, the pair $(*, A)$ can be understood as a locally ringed space. With A the algebra of formal power series $\mathbb{k}[[t]]$ over one variable t , this example plays an important role in the theory of formal deformations of algebras.

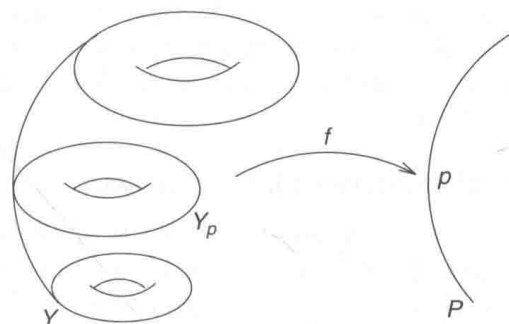


Figure 1 A fibered space.

Definition 3 A morphism $(f, \varphi): (Y, \mathcal{B}) \rightarrow (P, \mathcal{S})$ of ringed spaces is called fibered, if the following conditions are fulfilled:

- (i) (P, \mathcal{S}) is a commutative locally ringed space;
- (ii) $f: Y \rightarrow P$ is surjective; and
- (iii) $\varphi_y: \mathcal{S}_{f(y)} \rightarrow \mathcal{B}_y$ maps $\mathcal{S}_{f(y)}$ into the center of \mathcal{B}_y for each $y \in Y$.

The fiber of (f, φ) over a point $p \in P$ then is the ringed space (Y_p, \mathcal{B}_p) defined by

$$Y_p = f^{-1}(p), \quad \mathcal{B}_p = \mathcal{B}_{|f^{-1}(p)} / \mathfrak{m}_p \mathcal{B}_{|f^{-1}(p)}$$

where \mathfrak{m}_p is the maximal ideal of \mathcal{S}_p which acts on $\mathcal{B}_{|f^{-1}(p)}$ via φ .

A fibered morphism of ringed spaces can be pictured in Figure 1.

Additionally to this intuitive picture, conditions (i)–(iii) imply that the stalks \mathcal{B}_y are central extensions of $\mathcal{B}_y / \mathfrak{m}_{f(y)} \mathcal{B}_y$ by $\mathcal{S}_{f(y)}$.

Definition 4 Let (P, \mathcal{S}) be a commutative locally ringed space over a field \mathbb{k} with P connected, let $*$ be a fixed point in P , and (X, \mathcal{A}) a \mathbb{k} -ringed space. A deformation of (X, \mathcal{A}) over the parameter space (P, \mathcal{S}) with distinguished point $*$ then is a fibered morphism $(f, \varphi): (Y, \mathcal{B}) \rightarrow (P, \mathcal{S})$ over \mathbb{k} together with an isomorphism $(i, \iota): (X, \mathcal{A}) \rightarrow (Y_*, \mathcal{B}_*)$ such that for all $p \in P$ and $y \in f^{-1}(p)$ the homomorphism $\varphi_y: \mathcal{S}_p \rightarrow \mathcal{B}_y$ is flat.

The condition of flatness in the definition of a deformation serves as a substitute for “local triviality” and works also in the presence of singularities. (see Palamodov (1990), section 3) for a discussion of this point.

In the remainder of this section, we provide a list of some of the most important deformation problems in mathematics, and show how these can be formulated within the above language.

Products of \mathbb{k} -Ringed Spaces

Let (X, \mathcal{A}) be any \mathbb{k} -ringed space and (P, \mathcal{S}) a \mathbb{k} -scheme. For any closed point $*$ in P , the product

$(X \times P, \mathcal{B}) = (X, \mathcal{A}) \times_k (P, \mathcal{S})$ then is a flat deformation of (X, \mathcal{A}) with distinguished point $*$. This can be seen easily from the fact that $\mathcal{B}_{(x,p)} = \mathcal{A}_x \otimes_k \mathcal{S}_p$ for every $x \in X$ and $p \in P$.

Families of Matrices as Deformations

Let (P, \mathcal{O}_P) be a complex space with distinguished point $*$ and $A_P: P \rightarrow \text{Mat}(n \times n, \mathbb{C})$ a holomorphic family of complex $n \times n$ matrices over P . By the following construction, A_P can be understood as a deformation, more precisely as a deformation of the matrix $A := A_P(*)$. Let Y be the graph of A_P in the product space $P \times \text{Mat}(n \times n, \mathbb{C})$ and $f: Y \rightarrow P$ be the restriction of the projection onto the first coordinate. Define the sheaf \mathcal{B} as the inverse image sheaf $f^{-1}\mathcal{S}$, and let φ be the sheaf morphism which for every $y \in Y$ is induced by the identity map $\varphi_y: \mathcal{S}_{f(y)} \rightarrow \mathcal{B}_y := \mathcal{S}_{f(y)}$. It is then immediately clear that (f, φ) is a deformation of the fiber $f^{-1}(*)$ and that this fiber coincides with the matrix A .

Now let A be an arbitrary complex $n \times n$ -matrix, and choose a $\text{GL}(n, \mathbb{C})$ -slice through A , that is, a submanifold P containing A which is transversal to the $\text{GL}(n, \mathbb{C})$ -orbit through A . Hereby, it is assumed that $\text{GL}(n, \mathbb{C})$ acts by the adjoint action on $\text{Mat}(n \times n, \mathbb{C})$. The family A_P given by the canonical embedding $P \hookrightarrow \text{Mat}(n \times n, \mathbb{C})$ now is a deformation of A . The germ of this deformation at $*$ is versal in the sense defined in the next section.

Deformation of a Scheme à la Grothendieck

Assume that (P, \mathcal{S}) is a connected scheme over k . A deformation of a scheme (X, \mathcal{A}) then is a deformation $(f, \varphi): (Y, \mathcal{B}) \rightarrow (P, \mathcal{S})$ in the sense defined above, together with the requirement that $f: Y \rightarrow P$ is a proper map, that is, $f^{-1}(K)$ is compact for every compact $K \subset P$. As a particular example, consider the k -scheme $Y = \text{Spec } k[x, y, t]/(xy - t)$. It gives rise to a fibration $Y \rightarrow \text{Spec } k[t]$, whose fibers Y_a with $a \in k$ are hyperbolas $xy = a$, when $a \neq 0$, and consist of the two axes $x=0$ and $y=0$, when $a=0$. For $k=\mathbb{R}$, this deformation can be illustrated as in Figure 2.

For further information on this and similar examples, see Hartshorne (1977), in particular example 3.3.2.

Deformation of a Complex Space

According to Grothendieck, one understands by a deformation of a complex space (X, \mathcal{A}) a morphism of complex spaces $(f, \varphi): (Y, \mathcal{B}) \rightarrow (P, \mathcal{S})$ which is both a proper flat morphism of complex spaces and a deformation of (X, \mathcal{A}) as a ringed space. In case (X, \mathcal{A}) and (P, \mathcal{S}) are complex manifolds and if P is

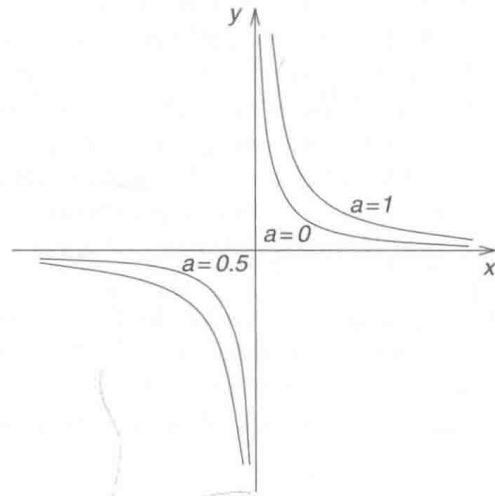


Figure 2 Deformation of the coordinate axes.

connected, each of the fibers Y_p is a compact complex manifold. Moreover, the family $(Y_p)_{p \in P}$ then is a family of compact complex manifolds in the sense of Kodaira–Spencer (cf. Palamodov (1990)).

Deformation of Singularities

Let p be a point of some \mathbb{C}^n . Two complex spaces $(X, \mathcal{O}_X) \subset (\mathbb{C}^n, \mathcal{O})$ and $(X', \mathcal{O}_{X'}) \subset (\mathbb{C}^n, \mathcal{O})$ with $x \in X \cap X'$ are then called germ equivalent at x if there exists an open neighborhood $U \in \mathbb{C}^n$ of x such that $X \cap U = X' \cap U$. Obviously, germ equivalence at x is an equivalence relation indeed. We denote the equivalence class of X by $[X]_x$. Clearly, if $[X]_x = [X']_x$, then one has $\mathcal{O}_{X,x} = \mathcal{O}_{X',x}$ for the stalks at x . By a singularity one understands a pair $([X]_x, \mathcal{O}_{X,x})$. In the literature, such a singularity is often denoted by (X, x) . The singularity (X, x) is called nonsingular or regular if $\mathcal{O}_{X,x}$ is isomorphic to an algebra of convergent power series $\mathbb{C}\{z_1, \dots, z_d\}$. A deformation of a complex singularity (X, x) over a complex germ $(P, *)$ is a morphism of ringed spaces $([Y]_x, \mathcal{O}_{Y,x}) \rightarrow ([P]_*, \mathcal{O}_{P,*})$ which is induced by a holomorphic map and which is a deformation of $([X]_x, \mathcal{O}_{X,x})$ as a ringed space. See Artin (1976) and the overview article by Greuel (1992) for further details and a variety of examples.

First-Order Deformation of Algebras

Consider a k -algebra A and the truncated polynomial algebra $S = k[\varepsilon]/\varepsilon^2 k[\varepsilon]$. Furthermore, let $\alpha: A \times A \rightarrow A$ be a Hochschild 2-cocycle of A ; in other words, assume that the relation

$$\begin{aligned} a_1 \alpha(a_2, a_3) - \alpha(a_1 a_2, a_3) + \alpha(a_1, a_2 a_3) \\ - \alpha(a_1, a_2) a_3 = 0 \end{aligned} \quad [1]$$

holds for all $a_1, a_2, a_3 \in A$. Then one can define a new k -algebra B , whose underlying linear structure

is isomorphic to $A \otimes_k S$ and whose product is given by the following construction: any element $b \in B$ can be written uniquely in the form $b = a_0 + a_1 \varepsilon$, with $a_0, a_1 \in A$. Then the product of $b = a_0 + a_1 \varepsilon \in B$ and $b' = a'_0 + a'_1 \varepsilon \in B$ is given by

$$b \cdot b' = a_0 a'_0 + [\alpha(a_0, a'_0) + a_0 a'_1 + a_1 a'_0] \varepsilon \quad [2]$$

By condition [1], this product is associative. One thus obtains a flat deformation $\Delta: S \rightarrow B$ of the algebra A and calls it the first-order or infinitesimal deformation of A along the Hochschild cocycle α . For further information on this and the connection between deformation theory and Hochschild cohomology, see the overview article by Gerstenhaber and Schack (1986).

Formal Deformation of an Algebra

Let us generalize the preceding example and explain the concept of a formal deformation of an algebra by Gerstenhaber. Assume again A to be an arbitrary k -algebra and choose bilinear maps $\alpha_n: A \times A \rightarrow A$ for $n \in \mathbb{N}$ such that α_0 is the product on A and α_1 is a Hochschild cocycle. Furthermore, let S be the algebra $k[[t]]$ of formal power series in one variable over k . Then define on the linear space $B = A[[t]]$ of formal power series in one variable with coefficients in A the following bilinear map:

$$\star: B \times B \rightarrow B$$

$$\left(\sum_{n \in \mathbb{N}} a_n t^n, \sum_{n \in \mathbb{N}} b_n t^n \right) \mapsto \sum_{n \in \mathbb{N}} \sum_{\substack{k, l \in \mathbb{N} \\ k+l=n}} \alpha_m(a_k, b_l) t^n \quad [3]$$

If B together with \star becomes a k -algebra or, in other words, if \star is associative, one can easily see that it gives a flat deformation of A over $S = k[[t]]$. In that case, one says that B is a formal deformation of A by the family $(\alpha_n)_{n \in \mathbb{N}}$. Contrarily to the preceding example, there might not exist for every Hochschild cocycle α on A a formal deformation B of A defined by a family $(\alpha_n)_{n \in \mathbb{N}}$ such that $\alpha_1 = \alpha$. In case it exists, we will say that the deformation B of A is in the direction of α . If the third Hochschild cohomology group $H^3(A, A)$ vanishes, there exists for every Hochschild cocycle α on A a deformation B of A in the direction of α (see again Gerstenhaber and Schack (1986) for further details).

Formal Deformation Quantization of Symplectic and Poisson Manifolds

Let us consider the last two examples for the case where A is the algebra $C^\infty(M)$ of smooth functions on a symplectic or Poisson manifold M . Then the Poisson bracket $\{, \}$ gives a Hochschild cocycle on $C^\infty(M)$. There exists a first-order deformation of $C^\infty(M)$ along

$(1/2i)\{, \}$ and, even though $HH^3(A, A)$ might not always vanish, a deformation quantization of M , that means a formal deformation of $C^\infty(M)$ in the direction of the Poisson bracket $(1/2i)\{, \}$. For the symplectic case, this fact has been proved first by deWilde–Lecomte using methods from Hochschild cohomology theory. A more geometric and intuitive proof has been given by Fedosov (1996). The Poisson case has been settled in the work of Kontsevich (2003) (see also the section “Deformation quantization of Poisson manifolds”).

Quantized Universal Enveloping Algebras According to Drinfel'd

A quantized universal enveloping algebra for a complex Lie algebra \mathfrak{g} is a Hopf algebra A over $\mathbb{C}[[t]]$ such that A is a topologically free $\mathbb{C}[[t]]$ -module (i.e., $A = (A/tA)[[t]]$ as left $\mathbb{C}[[t]]$ -module) and A/tA is the universal enveloping algebra $U\mathfrak{g}$ of \mathfrak{g} . Because A is a topologically free $\mathbb{C}[[t]]$ -module, A is a flat $\mathbb{C}[[t]]$ -module and thus a deformation of $U\mathfrak{g}$ over $\mathbb{C}[[t]]$. See Drinfel'd (1986) and the monograph by Kassel (1995) for further details and examples of quantized universal enveloping algebras.

Quantum Plane

Consider the tensor algebra $T = \bigoplus_{n \in \mathbb{N}} (\mathbb{R}^2)^{\otimes n}$ of the two-dimensional real vector space \mathbb{R}^2 , and let (x, y) be the canonical basis of \mathbb{R}^2 . Then form the tensor product sheaf $\mathcal{T}_{C^*} = T \otimes_{\mathbb{R}} \mathcal{O}_{C^*}$ and let \mathcal{I}_{C^*} be the ideal sheaf in \mathcal{T}_{C^*} generated by the relation

$$x \otimes y - zy \otimes x = 0 \quad [4]$$

where $z: C^* \rightarrow C$ is the identity function. The quotient sheaf $\mathcal{B} = \mathcal{B}_{C^*} = \mathcal{T}_{C^*} / \mathcal{I}_{C^*}$ then is a sheaf of C -algebras and an \mathcal{O}_{C^*} -module. Using eqn [4] now move all occurrences of x in an element of \mathcal{B}_{C^*} to the right of all y 's. Since $1/z$ is an element of $\mathcal{O}(C^*)$, one can thus show that \mathcal{B}_{C^*} is a free \mathcal{O}_{C^*} -module. Hence, \mathcal{B}_{C^*} is flat over \mathcal{O}_{C^*} . Further, it is easy to see that for every $q \in C^*$ the C -algebra $A_q = \mathcal{B}_q / \mathfrak{m}_q \mathcal{B}_q$ is freely generated by elements x, y with relations

$$x \otimes y - qy \otimes x = 0 \quad [5]$$

We call A_q the q -deformed quantum plane and $B = \mathcal{B}(C^*)$ the over C^* universally deformed quantum plane. Altogether, one can interpret B as a deformation of A_q over C^* , in particular as a deformation of $A_1 = T \otimes_{\mathbb{R}} C = C[x, y]$, the algebra of complex polynomials in two generators.

In the same way, one can deform function algebras on higher-dimensional vector spaces as well as function algebras on certain Lie groups. In this manner, one obtains the quantum group

$SU_q(2)$ as a deformation of a Hopf algebra of functions on $SU(2)$. See, for example, the work of Faddeev–Reshetikhin–Takhtajan (1990), Manin (1988) and Wess–Zumino (1990) for more information on q -deformations of vector spaces, Lie groups, differential calculi, etc.

Versal Deformations

In this section, and the ones that follow, we consider only germs of deformations, that is, deformations over parameter spaces of the form $(*, S)$. This means in particular that the structure sheaf only consists of its stalk S at $*$, a commutative local k -algebra. Let us now suppose that the sheaf morphism $\varphi: (Y, \mathcal{B}) \rightarrow (*, S)$ (over the canonical map $Y \rightarrow *$) is a deformation of the ringed space (X, \mathcal{A}) and that $\tau: T \rightarrow S$ is a homomorphism of commutative local k -algebras. Then the sheaf morphism $\tau^*\varphi: \mathcal{B} \otimes_S T \rightarrow T$ with $(\tau^*\varphi)_y(t) = 1 \otimes t$ for $y \in Y$ and $t \in T$ is a deformation of (X, \mathcal{A}) over the parameter space $(*, T)$. One says that the deformation $\tau^*\varphi$ is induced by the homomorphism τ .

Definition 5 A deformation $\varphi: (Y, \mathcal{B}) \rightarrow S$ of (X, \mathcal{A}) is called versal if every (germ of a) deformation of (X, \mathcal{A}) is isomorphic to a deformation germ induced by a homomorphism of k -algebras $\tau: T \rightarrow S$. A versal deformation is called universal, if the inducing homomorphism $\tau: T \rightarrow S$ is unique, and *miniversal* if S is of minimal dimension.

Example 6

- (i) In the section “Families of matrices as deformations,” the construction of a versal deformation of a complex matrix A has been sketched.
- (ii) According to Kuranishi, every compact complex manifold has a versal deformation by an analytic germ. See Kuranishi (1971) for a detailed exposition and the section “The Kodaira–Spencer algebra controlling deformations of compact complex manifolds” for a description of the principal ideas.
- (iii) Grauert has shown that for isolated singularities there exists a versal analytic deformation.
- (iv) By the work of Douady–Verdier, Grauert, and Palamodov one knows that for every compact complex space there exists a miniversal analytic deformation. One of the essential methods in the existence proof hereby is Palamodov’s construction of the cotangent complex (see Palamodov (1990)).
- (v) Bingener (1987) has further established Palamodov’s approach and thus has provided a

unified and quite general method for constructing versal deformations in analytic geometry.

- (vi) Fialowski–Fuchs have constructed miniversal deformations of Lie algebras.

Schlessinger’s Theorem

According to Grothendieck, spaces in algebraic geometry are represented by functors from a category of commutative rings to the category of sets. In this picture, an affine algebraic variety X over the base field k and with coordinate ring A is equivalently described by the functor $\text{Hom}_{\text{alg}}(A, -)$ defined on the category of commutative k -algebras. As will be shown by examples in the next section, versal deformations are often encoded by functors representing spaces. More precisely, a deformation problem leads to a so-called functor of Artin rings, which means a covariant functor F from the category of (local) Artinian k -algebras to the category of sets such that the set $F(k)$ has exactly one element. The question now arises as to under which conditions the functor F is representable, that is, there exists a commutative k -algebra A such that $F \cong \text{Hom}_{\text{alg}}(A, -)$. In the work of Schlessinger (1968), the structure of functors of Artin rings has been studied in detail. Moreover, criteria have been established, when such a functor is pro-presentable, which means that it can be represented by a complete local algebra \hat{A} , where “completeness” is understood with respect to the \mathfrak{m} -adic topology. Because of its importance for deformation theory, we will state Schlessinger’s theorem in this section. Before we come to its details, let us recall some notation.

Definition 7 By an Artinian k -algebra over a field k one understands a commutative k -algebra R which satisfies the following descending chain condition:

- (Dec) Every descending chain $I_1 \supset \dots \supset I_k \supset I_{k+1} \supset \dots$ of ideals in R becomes stationary.

Among others, an Artinian algebra R has the following properties:

1. R is Noetherian, that is, it satisfies the ascending chain condition.
2. Every prime ideal in R is maximal.
3. (Chinese remainder theorem) R is isomorphic to a finite product $\prod_{i=1}^n R_i$, where each R_i is a local Artinian algebra.
4. Every maximal ideal \mathfrak{m} of R is nilpotent, that is, $\mathfrak{m}^k = 0$ for some $k \in \mathbb{N}$.
5. Every quotient R/\mathfrak{m}^k with \mathfrak{m} maximal is finite dimensional.

Definition 8 Assume that $f: B \rightarrow A$ is a surjective homomorphism in the category $\mathbf{k}\text{-Alg}_{\text{Art}}$ of local Artinian \mathbf{k} -algebras. Then f is called a small extension if $\ker f$ is a nonzero principal ideal (b) in B such that $mb = (0)$, where m is the maximal ideal of B .

Theorem 9 (Schlessinger (1968, theorem 2.11)). Let F be a functor of Artin rings (over the base field \mathbf{k}). Assume that $A' \rightarrow A$ and $A'' \rightarrow A$ are morphisms in $\mathbf{k}\text{-Alg}_{\text{Art}}$, and consider the map

$$F(A' \times_A A'') \rightarrow F(A') \times_{F(A)} F(A'') \quad [6]$$

Then F is pro-representable if and only if F has the following properties:

- (H1) The map [6] is a surjection whenever $A'' \rightarrow A$ is a small extension.
- (H2) The map [6] is a bijection, when $A = \mathbf{k}$ and $A'' = \mathbf{k}[\varepsilon]$.
- (H3) One has $\dim_{\mathbf{k}}(t_F) < \infty$ for the tangent space $t_F := F(\mathbf{k}[\varepsilon])$.
- (H4) For every small extension $A' \rightarrow A$, the map

$$F(A' \times_A A') \rightarrow F(A') \times_{F(A)} F(A')$$

is an isomorphism.

Suppose that the functor F satisfies conditions (H1)–(H4), and let \hat{A} be an arbitrary complete local \mathbf{k} -algebra. By Yoneda's lemma, every element

$$\xi = \text{proj} \lim_{n \in \mathbb{N}} \xi_n \in \hat{A} = \text{proj} \lim_{n \in \mathbb{N}} \hat{A}/m^n \hat{A}$$

induces a natural transformation

$$\text{Hom}_{\text{alg}}(\hat{A}, -) \rightarrow F, \quad (u: \hat{A} \rightarrow R) \mapsto F(u_n)(\xi_n) \quad [7]$$

where $n \in \mathbb{N}$ is chosen large enough such that the homomorphism $u: \hat{A} \rightarrow R$ factors through some $u_n: \hat{A}/m^n \rightarrow R$. This is possible indeed, since R is Artinian. In the course of the proof of Schlessinger's theorem, \hat{A} and the element $\xi \in \hat{A}$ are now constructed in such a way that [7] is an isomorphism.

Differential Graded Lie Algebras and Deformation Problems

According to a philosophy going back to Deligne “every deformation problem in characteristic zero is controlled by a differential graded Lie algebra, with quasi-isomorphic differential graded Lie algebras giving the same deformation theory” (cf. Goldman and Millson (1988), p. 48). In the following, we will explain the main idea of this concept and apply it to two particular examples.

Differential Graded Lie Algebras

Definition 10 By a graded algebra over a field \mathbf{k} one understands a graded \mathbf{k} -vector space $A^\bullet = \bigoplus_{k \in \mathbb{Z}} A^k$ together with a bilinear map

$$\mu: A^\bullet \times A^\bullet \rightarrow A^\bullet, \quad (a, b) \mapsto a \cdot b = \mu(a, b)$$

such that $A^k \cdot A^l \subset A^{k+l}$ for all $k, l \in \mathbb{Z}$. The graded algebra A^\bullet is called associative if $(ab)c = a(bc)$ for all $a, b, c \in A^\bullet$.

A graded subalgebra of A^\bullet is a graded subspace $B^\bullet = \bigoplus_{k \in \mathbb{Z}} B^k \subset A^\bullet$ which is closed under μ , a graded ideal is a graded subalgebra $I^\bullet \subset A^\bullet$ such that $I^\bullet \cdot A^\bullet \subset I^\bullet$ and $A^\bullet \cdot I^\bullet \subset I^\bullet$.

A homomorphism between graded algebras A^\bullet and B^\bullet is a homogeneous map $f: A^\bullet \rightarrow B^\bullet$ of degree 0 such that $f(a \cdot b) = f(a) \cdot f(b)$ for all $a, b \in A^\bullet$.

From now on, assume that \mathbf{k} has characteristic $\neq 2, 3$. A graded Lie algebra then is a graded \mathbf{k} -vector space $\mathfrak{g}^\bullet = \bigoplus_{k \in \mathbb{Z}} \mathfrak{g}^k$ together with a bilinear map

$$[\cdot, \cdot]: \mathfrak{g}^\bullet \times \mathfrak{g}^\bullet \rightarrow \mathfrak{g}^\bullet, \quad (a, b) \mapsto [a, b]$$

such that the following axioms hold true:

1. $[\mathfrak{g}^k, \mathfrak{g}^l] \subset \mathfrak{g}^{k+l}$ for all $k, l \in \mathbb{Z}$.
2. $[\xi, \zeta] = -(-1)^{kl}[\zeta, \xi]$ for all $\xi \in \mathfrak{g}^k, \zeta \in \mathfrak{g}^l$.
3. $(-1)^{k_1 k_3} [[\xi_1, \xi_2], \xi_3] + (-1)^{k_2 k_1} [[\xi_2, \xi_3], \xi_1] + (-1)^{k_3 k_2} [[\xi_3, \xi_1], \xi_2] = 0$ for all $\xi_i \in \mathfrak{g}^{k_i}$ with $i = 1, 2, 3$.

By axiom (1), it is clear that a graded Lie algebra is in particular a graded algebra. So the above-defined notions of a graded ideal, homomorphism, etc., apply as well to graded Lie algebras.

Example 11 Let $A^\bullet = \bigoplus_{k \in \mathbb{Z}} A^k$ be a graded associative algebra. Then A^\bullet becomes a graded Lie algebra with the bracket

$$[a, b] = ab - (-1)^{kl}ba \quad \text{for } a \in A^k \text{ and } b \in A^l$$

The space A^\bullet regarded as a graded Lie algebra is often denoted by $\text{lie}^\bullet(A^\bullet)$.

Definition 12 A linear map $D: A^\bullet \rightarrow A^\bullet$ defined on a graded algebra A^\bullet is called a *derivation* of degree l if

$$D(ab) = (Da)b + (-1)^{kl}a(Db) \quad \text{for all } a \in A^k \text{ and } b \in A^l$$

A graded (Lie) algebra A^\bullet together with a derivation d of degree 1 is called a differential graded (Lie) algebra if $d \circ d = 0$. Then (A^\bullet, d) becomes a cochain complex. Since $\ker d$ is a graded

subalgebra of A^\bullet and $\text{im } d$ a graded ideal in $\ker d$, the cohomology space

$$H^\bullet(A^\bullet, d) = \ker d / \text{im } d$$

inherits the structure of a graded (Lie) algebra from A^\bullet .

Let $f: A^\bullet \rightarrow B^\bullet$ be a homomorphism of differential graded (Lie) algebras (A^\bullet, d) and (B^\bullet, ∂) . Assume further that f is a cochain map, that is, that $f \circ d = \partial \circ f$. Then one says that f is quasi-isomorphism or that the differential graded (Lie) algebras A^\bullet and B^\bullet are quasi-isomorphic if the induced homomorphism on the cohomology level $\bar{f}: H^\bullet(A^\bullet, d) \rightarrow H^\bullet(B^\bullet, \partial)$ is an isomorphism. Finally, a differential graded (Lie) algebra (A^\bullet, d) is called formal if it is quasi-isomorphic to its cohomology $(H^\bullet(A^\bullet, d), 0)$.

Maurer–Cartan Equation

Assume that $(\mathfrak{g}^\bullet, [\cdot, \cdot], d)$ is a differential graded Lie algebra over \mathbb{C} . Define the space $\mathcal{MC}(\mathfrak{g}^\bullet)$ of solutions of the Maurer–Cartan equation by

$$\mathcal{MC}(\mathfrak{g}^\bullet) := \{\omega \in \mathfrak{g}^1 \mid d\omega - \frac{1}{2}[\omega, \omega] = 0\} \quad [8]$$

In case the differential graded Lie algebra \mathfrak{g}^\bullet is nilpotent, this space naturally possesses a groupoid structure or, in other words, a set of arrows which are all invertible. The reason for this is that, under the assumption of nilpotency, the space \mathfrak{g}^0 is equipped with the Campbell–Hausdorff multiplication

$$\mathfrak{g}^0 \times \mathfrak{g}^0 \rightarrow \mathfrak{g}^0, \quad (X, Y) \mapsto \log(\exp X, \exp Y)$$

and the group \mathfrak{g}^0 acts on \mathfrak{g}^1 by the exponential function. More precisely, in this situation one can define for two objects $\alpha, \beta \in \mathcal{MC}(\mathfrak{g}^\bullet)$ the space of arrows $\alpha \rightarrow \beta$ as the set of all $\lambda \in \mathfrak{g}^0$ such that $\exp \lambda \cdot \alpha = \beta$.

We have now the means to define for every complex differential graded Lie algebra \mathfrak{g}^\bullet its deformation functor $\text{Def}_{\mathfrak{g}^\bullet}$. This functor maps the category of local Artinian \mathbb{C} -algebras to the category of groupoids and is defined on objects as follows:

$$\text{Def}_{\mathfrak{g}^\bullet}(R) := \mathcal{MC}(\mathfrak{g}^\bullet \otimes \mathfrak{m}) \quad [9]$$

Hereby, R is a complex local Artinian algebra, and \mathfrak{m} its maximal ideal. Note that since R is Artinian, $\mathfrak{g}^\bullet \otimes \mathfrak{m}$ is a nilpotent differential graded Lie algebra, hence $\text{Def}_{\mathfrak{g}^\bullet}(R)$ carries a groupoid structure as constructed above. Clearly, $\text{Def}_{\mathfrak{g}^\bullet}$ is also a functor of Artin rings as defined in the previous section.

With appropriate choices of the differential graded Lie algebra \mathfrak{g}^\bullet , essentially all deformation problems from the section “Basic definitions and examples” can be recovered via a functor of the

form $\text{Def}_{\mathfrak{g}^\bullet}$. Below, we will show in some detail how this works for two examples, namely the deformation theory of complex manifolds and the deformation quantization of Poisson manifolds. But before we come to this, let us state a result which shows how the deformation functor behaves under quasi-isomorphisms of the underlying differential graded Lie algebra. This result is crucial in a sense that it allows to equivalently describe a deformation problem with controlling \mathfrak{g}^\bullet by any other differential graded Lie algebra within the quasi-isomorphism class of \mathfrak{g}^\bullet . So, in particular in the case where the differential graded Lie algebra is formal, one often obtains a direct solution of the deformation problem.

Theorem 13 (Deligne, Goldman–Millson). *Assume that $f: \mathfrak{g}^\bullet \rightarrow \mathfrak{h}^\bullet$ is a quasi-isomorphism of differential graded Lie algebras. For every local Artinian \mathbb{C} -algebra R the induced functor $f_*: \text{Def}_{\mathfrak{g}^\bullet}(R) \rightarrow \text{Def}_{\mathfrak{h}^\bullet}(R)$ then is an equivalence of groupoids.*

The Kodaira–Spencer Algebra Controlling Deformations of Compact Complex Manifolds

Let M be a compact complex n -dimensional manifold. Recall that then the complexified tangent bundle $T_{\mathbb{C}}M$ has a decomposition into a holomorphic tangent bundle $T^{1,0}M$ and an antiholomorphic tangent bundle $T^{0,1}M$. This leads to a decomposition of the space of complex n -forms into the spaces $\Omega^{p,q}M$ of forms on M of type (p, q) . More generally, a smooth subbundle $J^{0,1} \subset T_{\mathbb{C}}M$ which induces a decomposition of the form $T_{\mathbb{C}}M = J^{1,0} \oplus J^{0,1}$, where $J^{1,0} := \overline{J^{0,1}}$, is called an almost complex structure on M . Clearly, the decomposition of $T_{\mathbb{C}}M$ into the holomorphic and antiholomorphic part is an almost complex structure, and an almost complex structure which is induced by a complex structure is called integrable. Assume that an almost complex structure $J^{0,1}$ is given on M and that it has finite distance to the complex structure on M . The latter means that the restriction $\varrho_j^{0,1}$ of the projection $\varrho: T_{\mathbb{C}}M \rightarrow T^{0,1}M$ along $T^{1,0}M$ to the subbundle $J^{0,1}$ is an isomorphism. Denote by β the inverse of $\varrho_j^{0,1}$, and let $\omega \in \Omega^{0,1}(M, T^{1,0}M)$ be the composition $-\varrho \circ \beta$. One checks immediately that every almost complex structure with finite distance to the complex structure on M is uniquely characterized by a section $\omega \in \Omega^{0,1}(M, T^{1,0}M)$ and that every element of $\Omega^{0,1}(M, T^{1,0}M)$ comes from an almost complex structure on M .

As a consequence of the Newlander–Nirenberg theorem, one can now show that the almost

complex structure $J^{0,1}$ resp. ω is integrable if and only if the equation

$$\bar{\partial}\omega - \frac{1}{2}[\omega, \omega] = 0 \quad [10]$$

is fulfilled. But this is nothing else than the Maurer–Cartan equation in the Kodaira–Spencer differential graded Lie algebra

$$(\mathfrak{Q}^\bullet, \bar{\partial}, [\cdot, \cdot]) = \left(\bigoplus_{p \in \mathbb{N}} \Omega^{0,p}(M, T^{1,0}M), \bar{\partial}, [\cdot, \cdot] \right)$$

Hereby, $\Omega^{0,p}(M, T^{1,0}M)$ denotes the $T^{1,0}M$ -valued differential forms on M of type $(0, p)$, $\bar{\partial}: \Omega^{0,p}(M, T^{1,0}M) \rightarrow \Omega^{0,p+1}(M, T^{1,0}M)$ the Dolbeault operator, and $[\cdot, \cdot]$ is induced by the Lie bracket of holomorphic vector fields. As a consequence of these considerations, deformations of the complex manifold M can equivalently be described by families $(\omega_p)_{p \in \mathbb{P}} \subset \mathfrak{Q}^1$ which satisfy eqn [10] and $\omega_* = 0$. Thus, it remains to determine the associated deformation functor $\text{Def}_{\mathfrak{Q}^\bullet}$.

According to Schlessinger's theorem, the functor $\text{Def}_{\mathfrak{Q}^\bullet}$ is pro-representable. Hence, there exists a local \mathbb{C} -algebra $R_{\mathfrak{Q}^\bullet}$ complete with respect to the \mathfrak{m} -adic topology such that

$$\text{Def}_{\mathfrak{Q}^\bullet}(R) = \text{Hom}_{\text{alg}}(R_{\mathfrak{Q}^\bullet}, R) \quad [11]$$

for every local Artinian \mathbb{C} -algebra R . Moreover, by Artin's theorem, there exists a “convergent” solution of the Maurer–Cartan equation, that is, $R_{\mathfrak{Q}^\bullet}$ can be replaced in eqn. [11] by a ring $\bar{R}_{\mathfrak{Q}^\bullet}$ representing an analytic germ.

Theorem 14 (Kodaira–Spencer, Kuranishi). *The ringed space $(\bar{R}_{\mathfrak{Q}^\bullet}, (0))$ is a miniversal deformation of the complex structure on M .*

Deformation Quantization of Poisson Manifolds

Let A be an associative \mathbb{k} -algebra with $\text{char } \mathbb{k} = 0$. Put for every integer $k \geq -1$

$$\mathfrak{g}^k := \text{Hom}_{\mathbb{k}}(A^{\otimes(k+1)}, A)$$

Then \mathfrak{g}^\bullet becomes a graded vector space. Let us impose a differential and a bracket on \mathfrak{g}^\bullet . The differential is the usual Hochschild coboundary $b: \mathfrak{g}^k \rightarrow \mathfrak{g}^{k+1}$,

$$\begin{aligned} bf(a_0 \otimes \cdots \otimes a_{k+1}) &:= a_0 f(a_1 \otimes \cdots \otimes a_{k+1}) \\ &+ \sum_{i=0}^k (-1)^{i+1} f(a_0 \otimes \cdots \otimes a_i a_{i+1} \otimes \cdots \otimes a_{k+1}) \\ &+ (-1)^k f(a_0 \otimes \cdots \otimes a_k) a_{k+1} \end{aligned}$$

The bracket is the Gerstenhaber bracket

$$\begin{aligned} [\cdot, \cdot] : \mathfrak{g}^{k_1} \times \mathfrak{g}^{k_2} &\rightarrow \mathfrak{g}^{k_1+k_2} \\ [f_1, f_2] &:= f_1 \circ f_2 - (-1)^{k_1 k_2} f_2 \circ f_1 \end{aligned}$$

where

$$\begin{aligned} f_1 \circ f_2(a_0 \otimes \cdots \otimes a_{k_1+k_2}) &:= \sum_{i=0}^{k_1} (-1)^{ik_2} f_1(a_0 \otimes \cdots \otimes a_{i-1} \otimes f_2(a_i \otimes \cdots \otimes a_{i+k_2}) \\ &\quad \otimes a_{i+k_2+1} \otimes \cdots \otimes a_{k_1+k_2}) \end{aligned}$$

The triple $(\mathfrak{g}^\bullet, b, [\cdot, \cdot])$ then is a differential graded Lie algebra.

Consider the Maurer–Cartan equation $b\gamma - (1/2)[\gamma, \gamma] = 0$ in \mathfrak{g}^1 . Obviously, it is equivalent to the equality

$$\begin{aligned} a_0 \gamma(a_1, a_2) - \gamma(a_0 a_1, a_2) + \gamma(a_0, a_1 a_2) - \gamma(a_0, a_1) a_2 \\ = \gamma(\gamma(a_0, a_1), a_2) - \gamma(a_0, \gamma(a_1, a_2)) \end{aligned} \quad [12]$$

for $a_0, a_1, a_2 \in A$

If one defines now for some $\gamma \in \mathfrak{g}^1$ the bilinear map $m: A \times A \rightarrow A$ by $m(a, b) = ab + \gamma(a, b)$, then [12] implies that m is associative if and only if γ satisfies the Maurer–Cartan equation.

Let us apply these observations to the case where A is the algebra $C^\infty(M)[[t]]$ of formal power series in one variable with coefficients in the space of smooth functions on a Poisson manifold M . By (a variant of) the theorem of Hochschild–Kostant–Rosenberg and Connes, one knows that in this case the cohomology of $(\mathfrak{g}^\bullet, b)$ is given by formal power series with coefficients in the space $\Gamma^\infty(\Lambda^\bullet TM)$ of antisymmetric vector fields. Now, $\Gamma^\infty(\Lambda^\bullet TM)$ carries a natural Lie algebra bracket as well, namely the Schouten bracket. Thus, one obtains a second differential graded Lie algebra $(\Gamma^\infty(\Lambda^\bullet TM)[[t]], 0, [\cdot, \cdot])$. Unfortunately, the projection onto cohomology $(\mathfrak{g}^\bullet, b) \rightarrow \Gamma^\infty(\Lambda^\bullet TM)[[t]]$ does not preserve the natural brackets, hence is not a quasi-isomorphism in the category of differential graded Lie algebras. It has been the fundamental observation by Kontsevich that this defect can be cured as follows.

Theorem 15 (Kontsevich 2003). *For every Poisson manifold M the differential graded Lie algebra $(\mathfrak{g}^\bullet, b, [\cdot, \cdot])$ is formal in the sense that there exists a quasi-isomorphism $(\mathfrak{g}^\bullet, b, [\cdot, \cdot]) \rightarrow (\Gamma^\infty(\Lambda^\bullet TM)[[t]], 0, [\cdot, \cdot])$ in the category of L^∞ -algebras.*

Note that the theorem only claims the existence of a quasi-isomorphism in the category of L^∞ -algebras or, in other words, in the category of homotopy Lie algebras. This is a notion somewhat weaker than a differential graded Lie algebra, but Theorem 13 also holds in the context of L^∞ -algebras.

Since the solutions of the Maurer–Cartan equation in $(\Gamma^\infty(\Lambda^*TM)[[t]], 0, [\cdot, \cdot])$ are exactly the formal paths of Poisson bivector fields on M , Kontsevich’s formality theorem entails:

Corollary 16 *Every Poisson manifold has a formal deformation quantization.*

See also: Deformation Quantization; Deformation Quantization and Representation Theory; Deformations of the Poisson Bracket on a Symplectic Manifold; Fedosov Quantization; Holonomic Quantum Fields; Operads.

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Deformations of the Poisson Bracket on a Symplectic Manifold

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Introduction to Deformation Quantization

The framework of classical mechanics, in its Hamiltonian formulation on the motion space, employs a symplectic manifold (or more generally a Poisson manifold). Observables are families of smooth functions on that manifold M . The dynamics is defined in terms of a Hamiltonian $H \in C^\infty(M)$ and the time evolution of an observable $f_t \in C^\infty(M \times \mathbb{R})$ is governed by the equation: $(d/dt)f_t = -\{H, f_t\}$.

The quantum-mechanical framework, in its usual Heisenberg’s formulation, employs a Hilbert space (states are rays in that space). Observables are families of self-adjoint operators on the Hilbert space. The dynamics is defined in terms of a Hamiltonian H , which is a self-adjoint operator,

and the time evolution of an observable A_t is governed by the equation $dA_t/dt = (i/\hbar)[H, A_t]$.

Quantization of a classical system is a way to pass from classical to quantum results. A first idea for quantization is to define a correspondence $Q: f \mapsto Q(f)$ mapping a function f to a self-adjoint operator $Q(f)$ on a Hilbert space \mathcal{H} in such a way that $Q(1) = \text{Id}$ and $[Q(f), Q(g)] = i\hbar Q(\{f, g\})$. Unfortunately, there is no such correspondence defined on all smooth functions on M when one puts an irreducibility requirement (which is necessary not to violate Heisenberg’s principle).

Different mathematical treatments of quantization have appeared:

- Geometric quantization of Kostant and Souriau: first, prequantization of a symplectic manifold (M, ω) where one builds a Hilbert space and a correspondence Q defined on all smooth functions on M but with no irreducibility; second, polarization to “cut down the number of variables.”
- Berezin’s quantization where one builds on a particular class of symplectic manifolds (some

Kähler manifolds) a family of associative algebras using a symbolic calculus, that is, a dequantization procedure.

- Deformation quantization introduced by Flato, Lichnerowicz, and Sternheimer in 1976 where they “suggest that quantization be understood as a deformation of the structure of the algebra of classical observables rather than a radical change in the nature of the observables.”

This deformation approach to quantization is part of a general deformation approach to physics (a seminal idea stressed by Flato): one looks at some level of a theory in physics as a deformation of another level.

Deformation quantization is defined in terms of a star product which is a formal deformation of the algebraic structure of the space of smooth functions on a Poisson manifold. The associative structure given by the usual product of functions and the Lie structure given by the Poisson bracket are simultaneously deformed.

In this article we concentrate on some mathematical results concerning deformations of the Poisson bracket on a symplectic manifold, classification of star products on symplectic manifolds, group actions on star products, convergence properties of some star products, and star products on cotangent bundles.

Deformations of the Poisson Bracket on a Symplectic Manifold

Definition 1 A Poisson bracket defined on the space of smooth functions on a manifold M is an \mathbb{R} -bilinear map on $C^\infty(M)$, $(u, v) \mapsto \{u, v\}$ such that for any $u, v, w \in C^\infty(M)$:

- (i) $\{u, v\} = -\{v, u\}$;
- (ii) $\{\{u, v\}, w\} + \{\{v, w\}, u\} + \{\{w, u\}, v\} = 0$;
- (iii) $\{u, vw\} = \{u, v\}w + \{u, w\}v$.

A Poisson bracket is given in terms of a contravariant skew-symmetric 2-tensor P on M (called the Poisson tensor) by $\{u, v\} = P(du \wedge dv)$. The Jacobi identity for the Poisson bracket is equivalent to the vanishing of the Schouten bracket $[P, P] = 0$. (The Schouten bracket is the extension – as a graded derivation for the exterior product – of the bracket of vector fields to skew-symmetric contravariant tensor fields.) A Poisson manifold (M, P) is a manifold M with a Poisson bracket defined by P .

A particular class of Poisson manifolds, essential in classical mechanics, is the class of “symplectic manifolds.” If (M, ω) is a symplectic manifold (i.e.,

ω is a closed nondegenerate 2-form on M) and if $u, v \in C^\infty(M)$, the Poisson bracket of u and v is

$$\{u, v\} := X_u(v) = \omega(X_v, X_u)$$

where X_u denotes the Hamiltonian vector field corresponding to the function u , that is, such that $i(X_u)\omega = du$. In coordinates the components of the Poisson tensor P^{ij} form the inverse matrix of the components ω_{ij} of ω .

Duals of Lie algebras form the class of linear Poisson manifolds. If \mathfrak{g} is a Lie algebra, then its dual \mathfrak{g}^* is endowed with the Poisson tensor P defined by $P_\xi(X, Y) := \xi([X, Y])$ for $X, Y \in \mathfrak{g} = (\mathfrak{g}^*)^* \sim (T_\xi \mathfrak{g}^*)^*$.

Definition 2 A Poisson deformation of the Poisson bracket on a Poisson manifold (M, P) is a Lie algebra deformation of $(C^\infty(M), \{, \})$ which is a derivation in each argument, that is, of the form $\{u, v\}_\nu = P_\nu(du, dv)$, where $P_\nu = P + \sum \nu^k P_k$ is a series of skew-symmetric contravariant 2-tensors on M (such that $[P_\nu, P_\nu] = 0$).

Two Poisson deformations P_ν and P'_ν of the Poisson bracket P on a Poisson manifold (M, P) are equivalent if there exists a formal path in the diffeomorphism group of M , starting at the identity, that is, a series $T = \exp D = \text{Id} + \sum_j (1/j!) D^j$ for $D = \sum_{r \geq 1} \nu^r D_r$ where the D_r are vector fields on M , such that

$$T\{u, v\}_\nu = \{Tu, Tv\}'_\nu$$

where $\{u, v\}_\nu = P_\nu(du, dv)$ and $\{u, v\}'_\nu = P'_\nu(du, dv)$.

Proposition 3 (Flato *et al.* 1975, Lecomte 1987). *On a symplectic manifold (M, ω) , any Poisson deformation of the Poisson bracket corresponds to a series of closed 2-forms on M , $\Omega_\nu = \omega + \sum_{r > 0} \nu^r \omega_r$ and is given by*

$$\{u, v\}_\nu = P_\nu(du, dv) = \Omega_\nu(X_u^\nu, X_v^\nu)$$

with $i(X_u^\nu)\Omega_\nu = du$. The equivalence classes of Poisson deformations of the Poisson bracket P are parametrized by $H^2(M; \mathbb{R})[[\nu]]$.

Poisson deformations are used in classical mechanics to express some constraints on the system. To deal with quantum mechanics, Flato *et al.* (1976) introduced star products. These give, by skew-symmetrization, Lie deformations of the Poisson bracket.

Definition 4 A “star product” on (M, P) is an $\mathbb{R}[[\nu]]$ -bilinear associative product $*$ on $C^\infty(M)[[\nu]]$ given by

$$u * v = u *_\nu v := \sum_{r \geq 0} \nu^r C_r(u, v)$$

for $u, v \in C^\infty(M)$ (we consider here real-valued functions; the results for complex-valued functions are similar), such that $C_0(u, v) = uv$, $C_1(u, v) - C_1(v, u) = \{u, v\}$, $1 * u = u * 1 = u$.

When the C_r 's are bidifferential operators on M , one speaks of a differential star product. When each C_r is a bidifferential operator of order at most r in each argument, one speaks of a natural star product.

One finds in the literature other normalizations for the skew-symmetric part of C_1 such as $(i/2)\{, \}$; these amount to a rescaling of the parameter ν . For physical applications, in the above convention for the formal parameter, ν corresponds to $i\hbar$, where \hbar is Planck's constant.

In the case of complex-valued functions, one can add the further requirement that the complex conjugation is a $*$ -involution for $*$, that is, $\overline{f * g} = \bar{g} * \bar{f}$. According to the interpretation of ν as being $i\hbar$, we have to require $\bar{\nu} = -\nu$. Star products satisfying this additional property are called symmetric or Hermitian.

A star product can also be defined not on the whole of $C^\infty(M)$ but on a subspace N which is stable under pointwise multiplication and Poisson bracket.

The simplest example of a deformation quantization is the Moyal product for the Poisson structure P on a vector space $V = \mathbb{R}^m$ with constant coefficients:

$$P = \sum_{i,j} P^{ij} \partial_i \wedge \partial_j, \quad P^{ij} = -P^{ji} \in \mathbb{R}$$

where $\partial_i = \partial/\partial y^i$ is the partial derivative in the direction of the coordinate y^i , $i = 1, \dots, n$. The formula for the Moyal product is

$$(u *_{\nu} v)(z) = \exp\left(\frac{\nu}{2} P^{rs} \partial_{y^r} \partial_{y'^s}\right) (u(y) \overline{v(y')})|_{y=y'=z} \quad [1]$$

When P is nondegenerate (so $V = \mathbb{R}^{2n}$), the space of formal power series of polynomials on V with Moyal product is called the formal Weyl algebra $W = (S(V)[[\nu]], *_M)$.

Let \mathfrak{g}^* be the dual of a Lie algebra \mathfrak{g} . The algebra of polynomials on \mathfrak{g}^* is identified with the symmetric algebra $S(\mathfrak{g})$. One defines a new associative law on this algebra by a transfer of the product \circ in the universal enveloping algebra $U(\mathfrak{g})$, via the bijection between $S(\mathfrak{g})$ and $U(\mathfrak{g})$ given by the total symmetrization σ :

$$\sigma : S(\mathfrak{g}) \rightarrow U(\mathfrak{g}) : X_1 \dots X_k \mapsto \frac{1}{k!} \sum_{\rho \in S_k} X_{\rho(1)} \circ \dots \circ X_{\rho(k)}$$

Then $U(\mathfrak{g}) = \bigoplus_{n \geq 0} U_n$, where $U_n := \sigma(S^n(\mathfrak{g}))$ and we decompose an element $u \in U(\mathfrak{g})$; accordingly $u = \sum u_n$. We define, for $P \in S^p(\mathfrak{g})$ and $Q \in S^q(\mathfrak{g})$,

$$P * Q = \sum_{n \geq 0} (\nu)^n \sigma^{-1}((\sigma(P) \circ \sigma(Q))_{p+q-n}) \quad [2]$$

This yields a differential star product on \mathfrak{g}^* (Gutt 1983). This star product can be written with an integral formula (for $\nu = 2\pi i$) (Drinfeld 1987):

$$u * v(\xi) = \int_{\mathfrak{g} \times \mathfrak{g}} \hat{u}(X) \hat{v}(Y) e^{2i\pi \langle \xi, \text{CBH}(X, Y) \rangle} dX dY$$

where $\hat{u}(X) = \int_{\mathfrak{g}^*} u(\eta) e^{-2i\pi \langle \eta, X \rangle}$ and CBH denotes Campbell–Baker–Hausdorff formula for the product of elements in the group in a logarithmic chart ($\exp X \exp Y = \exp \text{CBH}(X, Y) \forall X, Y \in \mathfrak{g}$). We call this the standard (or CBH) star product on the dual of a Lie algebra.

De Wilde and Lecomte (1983) proved that on any symplectic manifold there exists a differential star product. Fedosov (1994) gave a recursive construction of a star product on a symplectic manifold (M, ω) constructing flat connections on the Weyl bundle. Omori *et al.* (1991) gave an alternative proof of existence of a differential star product on a symplectic manifold, gluing local Moyal star products. In 1997, Kontsevich gave a proof of the existence of a star product on any Poisson manifold and gave an explicit formula for a star product for any Poisson structure on $V = \mathbb{R}^m$. This appeared as a consequence of the proof of his formality theorem.

Fedosov's Construction of Star Products

Fedosov's construction gives a star product on a symplectic manifold (M, ω) , when one has chosen a symplectic connection and a sequence of closed 2-forms on M . The star product is obtained by identifying the space $C^\infty(M)[[\nu]]$ with an algebra of flat sections of the so-called Weyl bundle endowed with a flat connection whose construction is related to the choice of the sequence of closed 2-forms on M .

Definition 5 The symplectic group $\text{Sp}(n, \mathbb{R})$ acts by automorphisms on the formal Weyl algebra W . If (M, ω) is a symplectic manifold, we can form its bundle $F(M)$ of symplectic frames which is a principal $\text{Sp}(n, \mathbb{R})$ -bundle over M . The associated bundle $\mathcal{W} = F(M) \times_{\text{Sp}(n, \mathbb{R})} W$ is a bundle of associative algebras on M called the Weyl bundle. Sections of the Weyl bundle have the form of formal series

$$a(x, y, \nu) = \sum_{2k+l \geq 0} \nu^k a_{(k) i_1 \dots i_l}(x) y^{i_1} \dots y^{i_l}$$

where the coefficients $a_{(k)}$ are symmetric covariant l -tensor fields on M . The product of two sections taken pointwise makes the space of sections into an algebra, and in terms of the above representation of sections the multiplication has the form

$$(a \circ b)(x, y, \nu) = \left(\exp \left(\frac{\nu}{2} P^{ij} \frac{\partial}{\partial y^i} \frac{\partial}{\partial z^j} \right) a(x, y, \nu) b(x, z, \nu) \right) \Big|_{y=z}$$

Note that the center of this algebra coincides with $C^\infty(M)[[\nu]]$.

A symplectic connection on M is a linear torsion-free connection ∇ such that $\nabla \omega = 0$.

Remark 6 It is well known that such connections always exist but, unlike the Riemannian case, are not unique. To see the existence, take any torsion-free connection ∇' and set $T(X, Y, Z) = (\nabla'_X \omega)(Y, Z)$. Define S by $\omega(S(X, Y), Z) = (1/3)(T(X, Y, Z) + T(Y, X, Z))$, then $\nabla_X Y = \nabla'_X Y + S(X, Y)$ defines a symplectic connection.

The connection ∇ induces a covariant derivative on sections of the Weyl bundle, denoted ∂ . The idea is to try to modify it to have zero curvature. Consider $Da = \partial a - \delta(a) - (1/\nu)[r, a]$, where r is a 1-form with values in \mathcal{W} , with $[a, a'dx] = (a \circ a' - a' \circ a)dx$ and $\delta(a) = (1/\nu)[\sum_{ij} \omega_{ij} y^i dx^j, a]$.

Theorem 7 (Fedosov 1994). *For a given series $\Omega = \sum_{i \geq 1} \nu^i \omega_i$ of closed 2-forms on M , there is a unique $r \in \Gamma(\mathcal{W} \otimes \Lambda^1)$ satisfying some normalization condition, so that $Da = \partial a - \delta(a) - (1/\nu)[r, a]$ is flat. For any $a_0 \in C^\infty(M)[[\nu]]$, there is a unique a in the subspace \mathcal{W}_D of flat sections of \mathcal{W} , such that $a(x, 0, \nu) = a_0(x, \nu)$. The use of this linear isomorphism to transport the algebra structure of \mathcal{W}_D to $C^\infty(M)[[\nu]]$ defines the star product of Fedosov $*_{\nabla, \Omega}$.*

Writing $*_{\nabla, \Omega} = \sum_{i \geq 0} \nu^i C_r^\Omega$, C_r^Ω only depends on ω_i for $i < r$ and $C_{r+1}^\Omega(u, \nu) = c\omega_r(X_u, X_\nu) + \tilde{C}_{r+1}(u, \nu)$, where $c \in \mathbb{R}$ and the last term does not depend on ω_r .

Classification of Star Products on a Symplectic Manifold

Star products on a manifold M are examples of deformations of associative algebras (in the sense of Gerstenhaber). Their study uses the Hochschild cohomology of the algebra (here $C^\infty(M)$ with values in $C^\infty(M)$) where p -cochains are p -linear maps from $(C^\infty(M))^p$ to $C^\infty(M)$ and where the Hochschild coboundary operator maps the p -cochain C to the $(p+1)$ -cochain

$$\begin{aligned} (\partial C)(u_0, \dots, u_p) &= u_0 C(u_1, \dots, u_p) \\ &+ \sum_{r=1}^p (-1)^r C(u_0, \dots, u_{r-1} u_r, \dots, u_p) \\ &+ (-1)^{p+1} C(u_0, \dots, u_{p-1}) u_p \end{aligned}$$

For differential star products, we consider differential cochains given by differential operators on each argument. The associativity condition for a star product at order k in the parameter ν reads

$$\begin{aligned} (\partial C_k)(u, v, w) &= \sum_{r+s=k, r, s > 0} (C_r(C_s(u, v), w) \\ &- C_r(u, C_s(v, w))) \end{aligned}$$

If one has cochains C_j , $j < k$ such that the star product they define is associative to order $k-1$, then the right-hand side above is a cocycle ($\partial(\text{RHS}) = 0$) and one can extend the star product to order k if it is a coboundary ($\text{RHS} = \partial(C_k)$).

Denoting by m the usual multiplication of functions, and writing $* = m + C$, where C is a formal series of multidifferential operators, the associativity also reads $\partial C = [C, C]$ where the bracket on the right-hand side is the graded Lie algebra bracket on $D_{\text{poly}}(M)[[\nu]] = \{\text{multidifferential operators}\}$.

Theorem 8 (Vey 1975). *Every differential p -cocycle C on a manifold M is the sum of the coboundary of a differential $(p-1)$ -cochain and a 1-differential skew-symmetric p -cocycle A : $C = \partial B + A$. In particular, a cocycle is a coboundary if and only if its total skew-symmetrization, which is automatically 1-differential in each argument, vanishes. Given a connection ∇ on M , B can be defined from C by universal formulas (Cahen and Gutt 1982). Also*

$$H_{\text{diff}}^p(C^\infty(M), C^\infty(M)) = \Gamma(\Lambda^p TM)$$

The similar result about continuous cochains is due to Connes (1985). In the somewhat pathological case of completely general cochains, the full cohomology is not known.

Definition 9 Two star products $*$ and $*'$ on (M, P) are said to be equivalent if there is a series of linear operators on $C^\infty(M)$, $T = \text{Id} + \sum_{r=1}^\infty \nu^r T_r$ such that

$$T(f * g) = T f *' T g \quad [3]$$

Remark that the T_r automatically vanish on constants since 1 is a unit for $*$ and for $*'$.

If $*$ and $*'$ are equivalent differential star products, then the equivalence is given by differential operators T_r ; if they are natural, the equivalence is given by $T = \text{Exp } E$ with $E = \sum_{r=1}^\infty \nu^r E_r$, where the E_r are differential operators of order at most $r+1$.

Nest and Tsygan (1995), then Deligne (1995) and Bertelson *et al.* (1995, 1997) proved that any differential star product on a symplectic manifold (M, ω) is equivalent to a Fedosov star product and that its equivalence class is parametrized by the corresponding element in $H^2(M; \mathbb{R})[[\nu]]$.

Kontsevich (IHES preprint 97) proved that the coincidence of the set of equivalence classes of star and Poisson deformations is true for general Poisson manifolds:

Theorem 10 (Kontsevich). *The set of equivalence classes of differential star products on a Poisson manifold (M, P) can be naturally identified with the set of equivalence classes of Poisson deformations of P : $P_\nu = P_0 + P_2\nu^2 + \dots \in \Gamma(X, \wedge^2 T_X)[[\nu]]$, $[P_\nu, P_\nu] = 0$.*

Deligne (1995) defines cohomological classes associated to differential star products on a symplectic manifold; this leads to an intrinsic way to parametrize the equivalence class of such a differential star product. The characteristic class $c(*)$ is given in terms of the skew-symmetric part of the term of order 2 in ν in the star product and in terms of local (“ ν -Euler”) derivations of the form $D = \nu(\partial/\partial\nu) + X + \sum_{r \geq 1} \nu^r D'_r$. This characteristic class has the following properties:

- The map C from equivalence classes of star products on (M, ω) to the affine space $-\omega/\nu + H^2(M; \mathbb{R})[[\nu]]$ mapping $[*]$ to $c(*)$ is a bijection.
- The characteristic class is natural relative to diffeomorphisms and is equivariant under a change of parameter (Gutt and Rawnsley 1995).
- The characteristic class $c(*)$ coincides (cf. Deligne (1995) and Neumaier (1999)) for Fedosov-type star products with their characteristic class introduced by Fedosov as the de Rham class of the curvature of the generalized connection used to build them (up to a sign and factors of 2).

Index theory has been introduced in the framework of deformation quantization by Fedosov (1996) and by Nest and Tsygan (1995, 1996). We refer to the papers of Bressler, Nest, and Tsygan for further developments in that subject. A first tool in that theory is the existence of a trace for the deformed algebra; this trace is essentially unique in the framework of symplectic manifolds (an elementary proof is given in Karabegov (1998) and Gutt and Rawnsley (2003)); the trace is not unique for more general Poisson manifolds.

Definition 11 A homomorphism from a differential star product $*$ on (M, P) to a differential star product $*'$ on (M', P') is an \mathbb{R} -linear map $A: C^\infty(M)[[\nu]] \rightarrow C^\infty(M')[[\nu]]$, continuous in the ν -adic topology, such that

$$A(u * v) = Au *' Av$$

It is an isomorphism if the map is bijective.

Any isomorphism between two differential star products on symplectic manifolds is the combination of a change of parameter and a ν -linear isomorphism. Any ν -linear isomorphism between two star products $*$ on (M, ω) and $*'$ on (M', ω') is the combination of the action on functions of a symplectomorphism $\psi: M' \rightarrow M$ and an equivalence between $*$ and the pullback via ψ of $*'$. It exists if and only if those two star products are equivalent, that is, if and only if $(\psi^{-1})^* c(*') = c(*)$, where $(\psi^{-1})^*$ denotes the action of ψ^{-1} on the second de Rham cohomology space. In particular, a symplectomorphism ψ of a symplectic manifold can be extended to a ν -linear automorphism of a given differential star product on (M, ω) if and only if $(\psi)^* c(*) = c(*)$ (Gutt and Rawnsley 1999).

The notion of homomorphism and its relation to modules has been studied by Bordemann (2004).

The link between the notion of star product on a symplectic manifold and symplectic connections already appears in the seminal paper of Bayen *et al.* (1978), and was further developed by Lichnerowicz (1982), who showed that any Vey star product (i.e., a star product defined by bidifferential operators whose principal symbols at each order coincide with those of the Moyal star product) determines a unique symplectic connection. Fedosov’s construction yields a Vey star product on any symplectic manifold starting from a symplectic connection and a formal series of closed 2-forms on the manifold. Furthermore, any star product is equivalent to a Fedosov star product and the de Rham class of the formal 2-form determines the equivalence class of the star product. On the other hand, many star products which appear in natural contexts (e.g., cotangent bundles or Kähler manifolds) are not Vey star products but are natural star products.

Theorem 12 (Gutt and Rawnsley 2004). *Any natural star product on a symplectic manifold (M, ω) determines uniquely*

- A symplectic connection $\nabla = \nabla(*)$.
- A formal series of closed 2-forms $\Omega = \Omega(*) \in \nu\Lambda^2(M)[[\nu]]$.
- A formal series $E = \sum_{r \geq 1} \nu^r E_r$ of differential operators of order $\leq r + 1$ (E_2 of order ≤ 2), with $E_r u = \sum_{k=2}^{r+1} (E_r^{(k)})^{i_1 \dots i_k} \nabla_{i_1 \dots i_k}^k u$, where the $E_r^{(k)}$ are symmetric contravariant k -tensor fields

such that

$$u * v = \exp -E((\exp Eu) *_{\nabla, \Omega} (\exp Ev)) \quad [4]$$

We denote $* = *_{\nabla, \Omega, E}$. If τ is a diffeomorphism of M then the data for $\tau * *$ is $\tau \cdot \nabla$, $\tau \cdot \Omega$, and $\tau \cdot E$. In

particular, a vector field X is a derivation of a natural star product $*$, if and only if $\mathcal{L}_X\omega=0$, $\mathcal{L}_X\Omega=0$, $\mathcal{L}_X\nabla=0$, and $\mathcal{L}_XE=0$.

Group Actions on Star Products

Symmetries in quantum theories are automorphisms of an algebra of observables. In the framework where quantization is defined in terms of a star product, a symmetry σ of a star product $*$ is an automorphism of the $\mathbb{R}[[\nu]]$ -algebra $C^\infty(M)[[\nu]]$ with multiplication given by $*$:

$$\sigma(u * v) = \sigma(u) * \sigma(v), \quad \sigma(1) = 1$$

where σ , being determined by what it does on $C^\infty(M)$, will be a formal series $\sigma(u) = \sum_{r \geq 0} \nu^r \sigma_r(u)$ of linear maps $\sigma_r: C^\infty(M) \rightarrow C^\infty(M)$. We denote by $\text{Aut}_{\mathbb{R}[[\nu]]}(M, *)$ the set of those symmetries.

Any such automorphism σ of $*$ then can be written as $\sigma(u) = T(u \circ \tau^{-1})$, where τ is a Poisson diffeomorphism of (M, P) and $T = \text{Id} + \sum_{r \geq 1} \nu^r T_r$ is a formal series of linear maps. If $*$ is differential, then the T_r are differential operators; if $*$ is natural, then $T = \text{Exp } E$ with $E = \sum_{r \geq 1} \nu^r E_r$ and E_r is a differential operator of order at most $r + 1$.

If σ_t is a one-parameter group of symmetries of the star product $*$, then its generator D will be a derivation of $*$. Denote the Lie algebra of ν -linear derivations of $*$ by $\text{Der}_{\mathbb{R}[[\nu]]}(M, *)$.

An action of a Lie group G on a star product $*$ on a Poisson manifold (M, P) is a homomorphism $\sigma: G \rightarrow \text{Aut}_{\mathbb{R}[[\nu]]}(M, *)$; then $\sigma_g = (\tau_g)^{-1*} + O(\nu)$ and there is an induced Poisson action τ of G on (M, P) .

Given a Poisson action τ of G on (M, P) , a star product is said to be "invariant" under G if all the $(\tau_g)^{-1*}$ are automorphisms of $*$.

An action of a Lie group G on $*$ induces a homomorphism of Lie algebras $D: \mathfrak{g} \rightarrow \text{Der}_{\mathbb{R}[[\nu]]}(M, *)$. For each $\xi \in \mathfrak{g}$, $D_\xi = \xi^* + \sum_{r \geq 1} \nu^r D_\xi^r$, where ξ^* is the fundamental vector field on M defined by τ ; hence,

$$\xi^*(x) = \frac{d}{dt} \Big|_0 \tau(\exp - t\xi)x$$

Such a homomorphism $D: \mathfrak{g} \rightarrow \text{Der}_{\mathbb{R}[[\nu]]}(M, *)$ is called an action of the Lie algebra \mathfrak{g} on $*$.

Proposition 13 (Arnal *et al.* 1983). *Given $D: \mathfrak{g} \rightarrow \text{Der}_{\mathbb{R}[[\nu]]}(M, *)$ a homomorphism so that for each $\xi \in \mathfrak{g}$, $D_\xi = \xi^* + \sum_{r \geq 1} \nu^r D_\xi^r$, where ξ^* are the fundamental vector fields on M defined by an action τ of G on M and the D_ξ^r are differential operators, then there exists a local homomorphism $\sigma: U \subset G \rightarrow \text{Aut}_{\mathbb{R}[[\nu]]}(M, *)$ so that $\sigma_* = D$.*

If we want the analog in our framework to the requirement that operators should correspond to the infinitesimal actions of a Lie algebra, we should ask the derivations to be inner so that functions are associated to the elements of the Lie algebra.

A derivation $D \in \text{Der}_{\mathbb{R}[[\nu]]}(M, *)$ is said to be essentially inner or Hamiltonian if $D = (1/\nu)\text{ad}_* u$ for some $u \in C^\infty(M)[[\nu]]$. We call an action of a Lie group almost $*$ -Hamiltonian if each D_ξ is essentially inner; this is equivalent to the knowledge of a linear map $\lambda: \mathfrak{g} \rightarrow C^\infty(M)[[\nu]]$ $\xi \mapsto \lambda_\xi$ so that $\text{ad}_*(1/\nu)[\lambda_\xi, \lambda_\eta]_* = \text{ad}_* \lambda_{[\xi, \eta]}$.

We say the action is $*$ -Hamiltonian if λ_ξ can be chosen to make

$$\mathfrak{g} \rightarrow C^\infty(M)[[\nu]], \quad \xi \mapsto \lambda_\xi$$

a homomorphism of Lie algebras, where $C^\infty(M)[[\nu]]$ is endowed with the bracket $(1/\nu)[,]_*$. Such a homomorphism is called a quantization in Arnal *et al.* (1983) and is called a generalized moment map in Bordemann *et al.* (1998).

When a map $\mu^0: \mathfrak{g} \rightarrow C^\infty(M)$ is a generalized moment map, that is,

$$\frac{1}{\nu} (\mu_\xi^0 * \mu_\eta^0 - \mu_\eta^0 * \mu_\xi^0) = \mu_{[\xi, \eta]}^0$$

the star product is said to be covariant under \mathfrak{g} .

When a map $\mu: \mathfrak{g} \rightarrow C^\infty(M)[[\nu]]$ is a generalized moment map, so that D_ξ has no terms in ν of degree > 0 , thus $D_\xi = \xi^*$, this map is called a quantum moment map (Xu 1998). Clearly in that situation, the star product is invariant under the action of \mathfrak{g} on M .

Covariant star products have been considered to study representations theory of some classes of Lie groups in terms of star products. In particular, an autonomous star formulation of the theory of representations of nilpotent Lie groups has been given by Arnal and Cortet (1984, 1985).

Consider a differential star product $*$ on a symplectic manifold, admitting an algebra \mathfrak{g} of vector fields on M consisting of derivations of $*$, and assume there is a symplectic connection ∇ which is invariant under \mathfrak{g} ; then $*$ is equivalent, through an equivariant equivalence (T with $\mathcal{L}_X T = 0$), to a Fedosov star product $*_{\nabla, \Omega}$; this yields to a classification of such invariant star products (Bertelson *et al.* 1998).

Proposition 14 (Kravchenko, Gutt and Rawnsley, Müller-Bahns, Neumaier, and Hamachi). *Consider a Fedosov star product $*_{\nabla, \Omega}$ on a symplectic manifold. A vector field X is a derivation of $*_{\nabla, \Omega}$ if and only if $\mathcal{L}_X\omega=0$, $\mathcal{L}_X\Omega=0$, and $\mathcal{L}_X\nabla=0$. A vector field X is an inner derivation of $*_{\nabla, \Omega}$ if*

and only if $\mathcal{L}_X \nabla = 0$ and there exists a series of functions λ_X such that

$$i(X)\omega - i(X)\Omega = d\lambda_X$$

In this case $X(u) = (1/\nu)(\text{ad}_* \lambda_X)(u)$.

On a symplectic manifold (M, ω) , a vector field X is an inner derivation of the natural star product $* = *_{\nabla, \Omega, E}$ if and only if $\mathcal{L}_X \nabla = 0$, $\mathcal{L}_X E = 0$, and there exists a series of functions λ_X such that

$$i(X)\omega - i(X)\Omega = d\lambda_X$$

Then $X = (1/\nu)\text{ad}_* \mu_X$ with $\mu_X = \text{Exp}(E^{-1})\lambda_X$.

Let G be a compact Lie group of symplectomorphisms of (M, ω) and \mathfrak{g} the corresponding Lie algebra of symplectic vector fields on M . Consider a star product $*$ on M which is invariant under G . The Lie algebra \mathfrak{g} consists of inner derivations for $*$ if and only if there exists a series of functions λ_X and a representative $(1/\nu)(\omega - \Omega)$ of the characteristic class of $*$ such that $i(X)\omega - i(X)\Omega = d\lambda_X$.

Star products which are invariant and covariant are used in the problem of reduction: this is a device in symplectic geometry which allows one to reduce the number of variables. An important issue in quantization is to know if and how quantization commutes with reduction. This problem has been studied by Fedosov for the action of a compact group on the particular star products constructed by him with trivial characteristic class $(*\nabla, 0)$. Here, one indeed obtains some “quantization commutes with reduction” statements. More generally, Bordemann, Herbig, and Waldmann considered covariant star products. In this case, one can construct a classical and quantum BRST complex whose cohomology describes the algebra of observables for the reduced system. While this is well known classically – at least under some regularity assumptions on the group action – for the quantized situation, the nontrivial question is whether the quantum BRST cohomology is “as large, as” the classical one. Clearly, from the physical point of view, this is crucial. It turns out that whereas for strongly invariant star products one indeed obtains a quantization of the reduced phase space, in general the quantum BRST cohomology might be too small. More general situations of reduction have also been discussed by, for example, Bordemann as well as Cattaneo and Felder, when a coisotropic (i.e., first class) constraint manifold is given.

Convergence of Some Star Products on a Subclass of Functions

Let (M, P) be a Poisson manifold and let $*$ be a differential star product on it with 1 acting as the identity. Observe that if there exists a value k of ν such that

$$u * v = \sum_{r=0}^{\infty} \nu^r C_r(u, v)$$

converges (for the pointwise convergence of functions), for all $u, v \in C^\infty(M)$, to $F_k(u, v)$ in such a way that F_k is associative, then $F_k(u, v) = uv$. This is easy to see as the order of differentiation in the C_r necessarily is at least r in each argument and thus the Borel lemma immediately gives the result. So assuming “too much” convergence kills all deformations. On the other hand, in any physical situation, one needs some convergence properties to be able to compute the spectrum of quantum observables in terms of a star product (as in Bayen *et al.* 1978).

In the example of Moyal star product on the symplectic vector space $(\mathbb{R}^{2n}, \omega)$, the formal formula

$$(u *_M v)(z) = \exp\left(\frac{\nu}{2} P^{rs} \partial_{x^r} \partial_{y^s}\right) (u(x)v(y)) \Big|_{x=y=z}$$

obviously converges when u and v are polynomials. On the other hand, there is an integral formula for Moyal star product given by

$$\begin{aligned} (u * v)(\xi) &= (\pi \hbar)^{-2n} \int u(\xi') v(\xi'') \\ &\quad \times \exp\left(\frac{2i}{\hbar} \left(\omega(\xi, \xi'') + \omega(\xi'' + \xi') \right. \right. \\ &\quad \left. \left. + \omega(\xi', \xi) \right) \right) d\xi' d\xi'' \end{aligned}$$

and this product $*$ gives a structure of associative algebra on the space of rapidly decreasing functions $\mathcal{S}(\mathbb{R}^{2n})$. The formal formula converges (for $\nu = i\hbar$) in the topology of \mathcal{S}' for u and v with compactly supported Fourier transform.

Some works have been done about convergence of star products.

- The method of quantization of Kähler manifolds due to Berezin as the inverse of taking symbols of operators, to construct on Hermitian symmetric spaces star products which are convergent on a large class of functions on the manifold (Moreno, Cahen Gutt, and Rawnsley, Karabegov, Schlichenmaier).

- The constructions of operator representations of star products (Fedosov, Bordemann, Neumaier, and Waldmann).
- The work of Rieffel and the notion of strict deformation quantization. Examples of strict (Fréchet) quantization have been given by Omori, Maeda, Niyazaki, and Yoshioka, and by Bieliavsky.

Convergence of Berezin-Type Star Products on Hermitian Symmetric Spaces

The method to construct a star product involves making a correspondence between operators and functions using coherent states, transferring the operator composition to the symbols, introducing a suitable parameter into this Berezin composition of symbols, taking the asymptotic expansion in this parameter on a large algebra of functions, and then showing that the coefficients of this expansion satisfy the cocycle conditions to define a star product on the smooth functions (Cahen *et al.* 1995). The idea of an asymptotic expansion appears in Berezin (1975) and in Moreno and Ortega-Navarro (1983, 1986).

This asymptotic expansion exists for compact M , and defines an associative multiplication on formal power series in k^{-1} with coefficients in $C^\infty(M)$ for compact coadjoint orbits. For M a Hermitian symmetric space of compact type and more generally for compact coadjoint orbits (i.e., flag manifolds), this formal power series converges on the space of symbols (Karabegov 1998).

For general Hermitian symmetric spaces of non-compact type, using their realization as bounded domains, one defines an analogous algebra of symbols of polynomial differential operators.

Reshetikhin and Takhtajan have constructed an associative formal star product given by an asymptotic expansion on any Kähler manifold. This they do in two steps, first building an associative product for which 1 is not a unit element, then passing to a star product.

We denote by (L, ∇, h) a quantization bundle for the Kähler manifold (M, ω, J) (i.e., a holomorphic line bundle L with connection ∇ admitting an invariant Hermitian structure h , such that the curvature is $\text{curv}(\nabla) = -2i\pi\omega$). We denote by \mathcal{H} the Hilbert space of square-integrable holomorphic sections of L which we assume to be nontrivial. The coherent states are vectors $e_q \in \mathcal{H}$ such that

$$s(x) = \langle s, e_q \rangle q, \quad \forall q \in \mathcal{L}_x, x \in M, s \in \mathcal{H}$$

(\mathcal{L} is the complement of the zero section in L). The function $\epsilon(x) = |q|^2 \|e_q\|^2, q \in \mathcal{L}_x$, is well defined and real analytic.

Let $A: \mathcal{H} \rightarrow \mathcal{H}$ be a bounded linear operator and let

$$\hat{A}(x) = \frac{\langle Ae_q, e_q \rangle}{\langle e_q, e_q \rangle}, \quad q \in \mathcal{L}_x, x \in M$$

be its symbol. The function \hat{A} has an analytic continuation to an open neighborhood of the diagonal in $M \times M$ given by

$$\hat{A}(x, y) = \frac{\langle Ae_{q'}, e_q \rangle}{\langle e_{q'}, e_q \rangle}, \quad q \in \mathcal{L}_x, q' \in \mathcal{L}_y$$

which is holomorphic in x and antiholomorphic in y . We denote by $\hat{E}(L)$ the space of symbols of bounded operators on \mathcal{H} . We can extend this definition of symbols to some unbounded operators provided everything is well defined.

The composition of operators on \mathcal{H} gives rise to an associative product $*$ for the corresponding symbols:

$$(\hat{A} * \hat{B})(x) = \int_M \hat{A}(x, y) \hat{B}(y, x) \psi(x, y) \epsilon(y) \frac{\omega^n(y)}{n!}$$

where

$$\psi(x, y) = \frac{|\langle e_{q'}, e_q \rangle|^2}{\|e_{q'}\|^2 \|e_q\|^2}, \quad q \in \mathcal{L}_x, q' \in \mathcal{L}_y$$

is a globally defined real analytic function on $M \times M$ provided ϵ has no zeros ($\psi(x, y) \leq 1$ everywhere, with equality where the lines spanned by e_q and $e_{q'}$ coincide).

Let k be a positive integer. The bundle $(L^k = \otimes^k L, \nabla^k, h^k)$ is a quantization bundle for $(M, k\omega, J)$ and we denote by \mathcal{H}^k the corresponding space of holomorphic sections and by $\hat{E}(L^k)$ the space of symbols of linear operators on \mathcal{H}^k . We let $\epsilon^{(k)}$ be the corresponding function. We say that the quantization is regular if $\epsilon^{(k)}$ is a nonzero constant for all non-negative k and if $\psi(x, y) = 1$ implies $x = y$. (Remark that if the quantization is homogeneous, all $\epsilon^{(k)}$ are constants.)

Theorem 15 (Cahen *et al.*). *Let (M, ω, J) be a Kähler manifold and (L, ∇, h) be a regular quantization bundle over M . Let \hat{A}, \hat{B} be in \mathcal{B} , where $\mathcal{B} \subset C^\infty(M)$ consists of functions f which have an analytic continuation in $M \times M$ so that $f(x, y) \psi(x, y)^l$ is globally defined, smooth and bounded on $K \times M$ and $M \times K$ for each compact subset K of M for some positive power l . Then*

$$(\hat{A} *_k \hat{B})(x) = \int_M \hat{A}(x, y) \hat{B}(y, x) \psi^k(x, y) \epsilon^{(k)} k^n \frac{\omega^n(y)}{n!}(y)$$

defined for k sufficiently large, admits an asymptotic expansion in k^{-1} as $k \rightarrow \infty$

$$(\hat{A} *_k \hat{B})(x) \sim \sum_{r \geq 0} k^{-r} C_r(\hat{A}, \hat{B})(x)$$

and the cochains C_r are smooth bidifferential operators, invariant under the automorphisms of the quantization and determined by the geometry alone. Furthermore, $C_0(\hat{A}, \hat{B}) = \hat{A}\hat{B}$ and $C_1(\hat{A}, \hat{B}) - C_1(\hat{B}, \hat{A}) = (i/\pi)\{\hat{A}, \hat{B}\}$.

If M is a flag manifold, this defines a star product on $C^\infty(M)$ and the $*_k$ product of two symbols is convergent (it is a rational function of k without pole at infinity) (cf. Karabegov in that generality).

If \mathcal{Q} be a bounded symmetric domain and \mathcal{E} the algebra of symbols of polynomial differential operators on a homogeneous holomorphic line bundle L over \mathcal{Q} which gives a realization of a holomorphic discrete series representation of G_0 , then for f and g in \mathcal{E} the Berezin product $f *_k g$ has an asymptotic expansion in powers of k^{-1} which converges to a rational function of k . The coefficients of the asymptotic expansion are bidifferential operators which define an invariant and covariant star product on $C^\infty(\mathcal{Q})$.

Star Products on Cotangent Bundles

Since from the physical point of view cotangent bundles $\pi: T^*Q \rightarrow Q$ over some configuration space Q , endowed with their canonical symplectic structure ω_0 , are one of the most important phase spaces, any quantization scheme should be tested and exemplified for this class of classical mechanical systems.

We first recall that on T^*Q there is a canonical vector field ξ , the Euler or Liouville vector field which is locally given by $\xi = p_k(\partial/\partial p_k)$. Here and in the following, we use local bundle coordinates (q^k, p_k) induced by local coordinates x^k on Q . Using ξ we can characterize those functions $f \in C^\infty(T^*Q)$ which are polynomial in the fibers of degree k by $\xi f = kf$. They are denoted by $\text{Pol}^k(T^*Q)$, whereas $\text{Pol}^\bullet(T^*Q)$ denotes the subalgebra of all functions which are polynomial in the fibers. Clearly, most of the physically relevant observables such as the kinetic energy, potentials, and generators of point transformations are in $\text{Pol}^\bullet(T^*Q)$. Moreover, $\text{Pol}^\bullet(T^*Q)$ is a Poisson subalgebra with

$$\{\text{Pol}^k(T^*Q), \text{Pol}^\ell(T^*Q)\} \subseteq \text{Pol}^{k+\ell-1}(T^*Q) \quad [5]$$

since $\mathcal{L}_\xi \omega_0 = \omega_0$ is conformally symplectic.

All this suggests that for a quantization of T^*Q , the polynomials $\text{Pol}^\bullet(T^*Q)$ should play a crucial role. In deformation quantization this is accomplished by the notion of a homogeneous star product (De Wilde and Lecomte 1983). If the operator

$$H = \nu \frac{\partial}{\partial \nu} + \mathcal{L}_\xi \quad [6]$$

is a derivation of a formal star product \star , then \star is called homogeneous. It immediately follows that $\text{Pol}(T^*Q)[\nu] \subseteq C^\infty(T^*Q)[[\nu]]$ is a subalgebra over the ring $C[[\nu]]$ of polynomials in ν . Hence for homogeneous star products, the question of convergence (in general quite delicate) has a simple answer.

Let us now describe a simple construction of a homogeneous star product (following Bordemann et al. (1998)). We choose a torsion-free connection ∇ on Q and consider the operator of the symmetrized covariant derivative, locally given by

$$D = dx^k \vee \nabla_{\partial/\partial x^k} : \Gamma^\infty(S^k T^*Q) \rightarrow \Gamma^\infty(S^{k+1} T^*Q) \quad [7]$$

Clearly, D is a global object and a derivation of the symmetric algebra $\bigoplus_{k=0}^\infty \Gamma^\infty(S^k T^*Q)$. Let now $f \in \text{Pol}^\bullet(T^*Q)$ and $\psi \in C^\infty(Q)$ be given. Then one defines the standard-ordered quantization $\varrho_{\text{Std}}(f)$ of f with respect to ∇ to be the differential operator $\varrho_{\text{Std}}(f) : C^\infty(Q) \rightarrow C^\infty(Q)$ locally given by

$$\begin{aligned} \varrho_{\text{Std}}(f)\psi &= \sum_{r=0}^\infty \frac{(-\nu)^r}{r!} \frac{1}{\partial p_{k_1} \cdots \partial p_{k_r}} \left|_{p=0} \frac{\partial f}{\partial x^{k_1} \cdots \partial x^{k_r}} \right| \\ &\times i_s \left(\frac{\partial}{\partial x^{k_1}} \right) \cdots i_s \left(\frac{\partial}{\partial x^{k_r}} \right) \frac{1}{r!} D^r \psi \quad [8] \end{aligned}$$

where i_s denotes the symmetric insertion of vector fields in symmetric forms. Again, this is independent of the coordinate system x^k . The infinite sum is actually finite as long as $f \in \text{Pol}^\bullet(T^*Q)$ whence we can safely set $\nu = i\hbar$ in this case. Indeed, [8] is the well-known symbol calculus for differential operators and it establishes a linear bijection

$$\varrho_{\text{Std}} : \text{Pol}^\bullet(T^*Q) \rightarrow \text{DiffOp}(C^\infty(Q)) \quad [9]$$

which generalizes the usual canonical quantization in the flat case of $T^*Q = T^*\mathbb{R}^n = \mathbb{R}^{2n}$. Using this linear bijection, we can define a new product \star_{Std} for $\text{Pol}^\bullet(T^*Q)$ by

$$f \star_{\text{Std}} g = \varrho_{\text{Std}}^{-1}(\varrho_{\text{Std}}(f)\varrho_{\text{Std}}(g)) = \sum_{r=0}^\infty \nu^r C_r(f, g) \quad [10]$$

It is now easy to see that \star_{Std} fulfills all requirements of a homogeneous star product except for the fact that the $C_r(\cdot, \cdot)$ are bidifferential. In this approach

this is far from being obvious as we only worked with functions polynomial in the fibers so far. Nevertheless, it is true whence \star_{Std} indeed defines a star product for $C^\infty(T^*Q)[[\nu]]$.

In fact, there is a different characterization of \star_{Std} using a slightly modified Fedosov construction: first one uses ∇ to define a torsion-free symplectic connection on T^*Q by a fairly standard lifting. Moreover, using ∇ one can define a standard-ordered fiberwise product \circ_{Std} for the formal Weyl algebra bundle over T^*Q , being the starting point of the Fedosov construction of star products. With these two ingredients one finally obtains \star_{Std} from the Fedosov construction with the big advantage that now the order of differentiation in the C_r can easily be determined to be r in each argument, whence \star_{Std} is even a natural star product. Moreover, C_r differentiates the first argument only in momentum directions which reflects the standard ordering.

Already in the flat situation the standard ordering is not an appropriate quantization scheme from the physical point of view as it maps real-valued functions to differential operators which are not symmetric in general. To pose this question in a geometric framework, we have to specify a positive density $\mu \in \Gamma^\infty(|\Lambda^n|T^*Q)$ on the configuration space Q first, as for functions there is no invariant meaning of integration. Specifying μ we can consider the pre-Hilbert space $C_0^\infty(Q)$ with inner product

$$\langle \phi, \psi \rangle = \int_Q \bar{\phi} \psi \mu \quad [11]$$

Now the adjoint with respect to [11] of $\varrho_{\text{Std}}(f)$ can be computed explicitly. We first consider the second-order differential operator

$$\Delta = \frac{\partial^2}{\partial q^k \partial p_k} + p_k \Gamma_{\ell m}^k \frac{\partial^2}{\partial p_\ell \partial p_m} + \Gamma_{k\ell}^k \frac{\partial}{\partial p_\ell} \quad [12]$$

where $\Gamma_{\ell m}^k$ are the Christoffel symbols of ∇ . In fact, Δ is defined independently of the coordinates and coincides with the Laplacian of the pseudo-Riemannian metric on T^*Q which is obtained from the natural pairing of vertical and horizontal spaces defined by using ∇ . Moreover, we need the 1-form α defined by $\nabla_X \mu = \alpha(X)\mu$ and the corresponding vertical vector field $\alpha^\vee \in \Gamma^\infty(T(T^*Q))$ locally given by $\alpha^\vee = \alpha_k(\partial/\partial p_k)$. Then

$$\varrho_{\text{Std}}(f)^\dagger = \varrho_{\text{Std}}(N^2 \bar{f}), \quad N = e^{(\nu/2)(\Delta + \alpha^\vee)} \quad [13]$$

Note that due to the curvature contributions, this statement is a highly nontrivial partial integration compared to the flat case. Note also that for

$f \in \text{Pol}(T^*Q)[\nu]$, we have $Nf \in \text{Pol}(T^*Q)[\nu]$ as well, and N commutes with H . As in the flat case this allows one to define a Weyl-ordered quantization by

$$\varrho_{\text{Weyl}}(f) = \varrho_{\text{Std}}(Nf) \quad [14]$$

together with a so-called Weyl-ordered star product

$$f \star_{\text{Weyl}} g = N^{-1}(Nf \star_{\text{Std}} Ng) \quad [15]$$

which is now a Hermitian and homogeneous star product such that ϱ_{Weyl} becomes a \star -representation of \star_{Weyl} , that is, we have $\varrho_{\text{Weyl}}(f \star_{\text{Weyl}} g) = \varrho_{\text{Weyl}}(f) \varrho_{\text{Weyl}}(g)$ and $\varrho_{\text{Weyl}}(f)^\dagger = \varrho_{\text{Weyl}}(\bar{f})$. Note that in the flat case this is precisely the Moyal star product \star_M from [1].

The star products \star_{Std} and \star_{Weyl} have been extensively studied by Bordemann, Neumaier, Pflaum, and Waldmann and provide now a well-understood quantization on cotangent bundles. We summarize a few highlights of this theory:

1. In the particular case of a Levi-Civita connection ∇ for some Riemannian metric g and the corresponding volume density μ_g , the 1-form α vanishes. This simplifies the operator N and describes the physically most interesting situation.
2. If the configuration space is a Lie group G , then its cotangent bundle $T^*G \cong G \times \mathfrak{g}^*$ is trivial by using, for example, left-invariant 1-forms. In this case the star products \star_{Weyl} and \star_{Std} restrict to the CBH star product on \mathfrak{g}^* . Moreover, \star_{Weyl} coincides with the star product found by Gutt (1983) on T^*G .
3. Using the operator N one can interpolate between the two different ordering descriptions ϱ_{Std} and ϱ_{Weyl} by inserting an additional ordering parameter κ in the exponent, that is, $N_\kappa = \exp(\nu\kappa(\Delta + \alpha^\vee))$. Thus, one obtains κ -ordered representations ϱ_κ together with corresponding κ -ordered star products \star_κ , where $\kappa=0$ corresponds to standard ordering and $\kappa=1/2$ corresponds to Weyl ordering. For $\kappa=1$, one obtains antistandard ordering and in general one has the relation $\bar{f} \star_\kappa g = \bar{g} \star_{1-\kappa} f$ as well as $\varrho_\kappa(f)^\dagger = \varrho_{1-\kappa}(\bar{f})$.
4. One can describe also the quantization of an electrically charged particle moving in a magnetic background field B . This is modeled by a closed 2-form $B \in \Gamma^\infty(\Lambda^2 T^*Q)$ on Q . Using local vector potentials $A \in \Gamma^\infty(T^*Q)$ with $B = dA$ locally, and by minimal coupling, one obtains a star product \star_B which depends only on B and not on the local potentials A . It will be equivalent to \star_{Weyl} if and only if B is exact. In general, its characteristic class is, up to a factor, given by the class $[B]$ of the magnetic field B . While the observable

algebra always exists, a Schrödinger-like representation of \star_B only exists if B satisfies the usual integrality condition. In this case, there exists a representation on sections of a line bundle whose first Chern class is given by $[B]$. This manifests Dirac's quantization condition for magnetic charges in deformation quantization. Another equivalent interpretation of this result is obtained by Morita theory: the star products \star_{Weyl} and \star_B are Morita equivalent if and only if B satisfies Dirac's integrality condition.

5. Analogously, one can determine the unitary equivalence classes of representations for a fixed, exact magnetic field B . It turns out that the representations depend on the choice of the global vector potential A and are unitarily equivalent if the difference between the two vector potentials satisfies an integrality condition known from the Aharonov–Bohm effect. This way, the Aharonov–Bohm effect can be formulated within the representation theory of deformation quantization.
6. There are several variations of the representations ϱ_{Std} and ϱ_{Weyl} . In particular, one can construct a representation on half-forms instead of functions, thereby avoiding the choice of the integration density μ . Moreover, all the Weyl-ordered representations can be understood as GNS representations coming from a particular positive functional, the Schrödinger functional. For ϱ_{Weyl} this functional is just the integration over the configuration space Q .
7. All the (formal) star products and their representations can be understood as coming from formal asymptotic expansions of integral formulas. From this point of view, the formal representations and

star products are a particular kind of global symbol calculus.

8. At least for a projectible Lagrangian submanifold L of T^*Q , one finds representations of the star product algebras on the functions on L . This leads to explicit formulas for the WKB expansion corresponding to this Lagrangian submanifold.
9. The relation between configuration space symmetries, the corresponding phase-space reduction, and the reduced star products has been analyzed extensively by Kowalzig, Neumaier, and Pflaum.

See also: Classical r -Matrices, Lie Bialgebras, and Poisson Lie Groups; Deformation Quantization; Deformation Quantization and Representation Theory; Deformation Theory; Fedosov Quantization; Operads.

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$\bar{\partial}$ -Approach to Integrable Systems

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Introduction

The $\bar{\partial}$ -approach is one of the most generic methods for constructing solutions of completely integrable systems. Taking into account that most soliton systems are represented as compatibility condition for a set of linear differential operators (Lax pairs, zero-curvature representations, L–A–B Manakov triples), it is sufficient to construct these operators.

Such compatible families can be defined by presenting their common eigenfunctions. If it is possible to show that some analytic constraints imply that a function is a common eigenfunction of a family of operators, solutions of original nonlinear system are also generated.

The main idea of the $\bar{\partial}$ method is to impose the following analytic constraints: if λ denotes the spectral parameter and x the physical variables, then, for arbitrary fixed values x , the $\partial_{\bar{\lambda}}$ derivative of the wave function is expressed as a linear combination of the wave functions at other values of λ with x -independent coefficients. In specific examples, this property is either derived from the

direct spectral transform or imposed *a priori*. Of course, the specific realization of this scheme depends critically on the nonlinear system.

The origin of the $\bar{\partial}$ -method came from the following observation. A solution of the one-dimensional inverse-scattering problem (the problem of reconstructing the potential by discrete spectrum and scattering amplitude at positive energies) for the one-dimensional time-independent Schrödinger operator

$$L = -\partial_x^2 + u(x) \quad [1]$$

was obtained by Gelfand, Levitan, and Marchenko in the 1950s. It essentially used analytic continuation of the wave function from the real momenta to the complex ones. If the potential $u(x)$ decays sufficiently fast as $|x| \rightarrow \infty$, then the eigenfunction equation

$$L\psi(k, x) = k^2\psi(k, x) \quad [2]$$

has two solutions $\psi_+(k, x)$ and $\psi_-(k, x)$ such that

1. $\psi_{\pm}(k, x) = (1 + o(1))e^{ikx}$ as $x \rightarrow \pm\infty$.
2. The functions $\psi_+(k, x), \psi_-(k, x)$ are holomorphic in k in the upper half-plane and the lower half-plane, respectively.

Existence of analytic continuation to complex momenta is typical for one-dimensional systems. But in the multidimensional case the situation is different. For example, wave functions for the multidimensional Schrödinger operator constructed by Faddeev are well defined for all complex momenta k , but they are nonholomorphic in k , and they become holomorphic only after restriction to some special one-dimensional subspaces. The last property was one of the key points in the Faddeev approach.

Beals and Coifman (1981–82) and Ablowitz *et al.* (1983) discovered that departure from holomorphicity for multidimensional wave functions can be interpreted as spectral data. Such spectral transforms proved to be very natural and suit perfectly the purposes of the soliton theory. Some other famous methods, including the Riemann–Hilbert problem, can be interpreted as special reductions of the $\bar{\partial}$ method.

Nonlocal $\bar{\partial}$ -Problem and Local $\bar{\partial}$ -Problem

The most generic formulation of the $\bar{\partial}$ -method is the nonlocal $\bar{\partial}$ -problem. Assume that the following data is given:

1. A rational $n \times n$ matrix-valued normalization function $\eta(\lambda)$.

2. An $n \times n$ matrix-valued function $g(\lambda, x)$ (it describes the dynamics) such that

- $g(\lambda, x)$ depends on the spectral parameter $\lambda \in \mathbb{C}$ and “physical” variables $x = (x_1, \dots, x_N)$; the physical variables x_k are either continuous (x_k belongs to a domain in \mathbb{R} or in \mathbb{C}) or discrete (x_k takes integer values);
- $g(\lambda, x)$ is analytic in λ , defined for all $\lambda \in \mathbb{C}$, except for a finite number of singular points, and is single valued; and
- $\det g(\lambda, x)$ has only finite number of zeros.

For problems with continuous physical variables the typical form of $g(\lambda, x)$ is $g(\lambda, x) = \exp(\sum_i x_i K_i(\lambda))$, where $K_i(\lambda)$ are meromorphic matrices, mutually commuting for all λ . The discrete variables are usually encoded in orders of poles and zeros.

3. An $n \times n$ matrix-valued function $R(\lambda, \mu)$ – the “generalized spectral data.” Usually, it is a regular function of four real variables $\Re\lambda, \Im\lambda, \Re\mu, \Im\mu$. (We write this as a function of two complex variables, but we do not assume it to be holomorphic. It would be more precise to write it as $R(\lambda, \bar{\lambda}, \mu, \bar{\mu})$, but to avoid long notations we omit the $\bar{\lambda}, \bar{\mu}$ dependence.) To avoid analytical complications, the function $R(\lambda, \mu)$ is usually assumed to vanish as λ or μ tend to singular points of $\eta(\lambda), g(\lambda, x)$.

Then the wave function Ψ is defined by the data using the following properties:

1. $\Psi = \Psi(\lambda, x)$ takes values in complex $n \times n$ matrices:

$$\Psi(\lambda, x) = \begin{bmatrix} \psi_{11}(\lambda, x) & \dots & \psi_{1n}(\lambda, x) \\ \vdots & \dots & \vdots \\ \psi_{n1}(\lambda, x) & \dots & \psi_{nn}(\lambda, x) \end{bmatrix} \quad [3]$$

2. For all $\lambda \in \mathbb{C}$ outside the singular points, the $\eta(\lambda), g(\lambda, x)$ wave function Ψ satisfies the $\bar{\partial}$ -equation of inverse-spectral problem,

$$\frac{\partial \Psi(\lambda, x)}{\partial \bar{\lambda}} = \iint_{\mu \in \mathbb{C}} d\mu \wedge d\bar{\mu} \Psi(\mu, x) R(\lambda, \mu) \quad [4]$$

It is important that condition [4] is x -independent.

3. The function $\chi(\lambda, x) - \eta(\lambda)$, where $\chi(\lambda, x) = \Psi(\lambda, x)g^{-1}(\lambda, x)$, is regular for all $\lambda \in \mathbb{C}$ and

$$\chi(\lambda, x) - \eta(\lambda) \rightarrow 0 \quad \text{as } |\lambda| \rightarrow \infty \quad [5]$$

The wave function $\Psi(\lambda, x)$ is calculated by employing the data $\eta(\lambda), g(\lambda, x), R(\lambda, \mu)$ using the following procedure. Taking into account that the

functions $\eta(\lambda)$, $g(\lambda, \mathbf{x})$ are holomorphic in λ , eqn [4] can be rewritten in terms of $\chi(\lambda, \mathbf{x})$:

$$\frac{\partial[\chi(\lambda, \mathbf{x}) - \eta(\lambda)]}{\partial \bar{\lambda}} = \iint_{\mu \in \mathbb{C}} d\mu \wedge d\bar{\mu} \chi(\mu, \mathbf{x}) g(\lambda, \mathbf{x}) \times R(\lambda, \mu) g^{-1}(\mu, \mathbf{x}) \quad [6]$$

The right-hand side of [6] is regular; therefore, this relation is valid for all complex λ values.

Equation [6] with the boundary condition [5] is equivalent to the following integral equation:

$$\begin{aligned} \chi(\lambda, \mathbf{x}) = & \eta(\lambda) + \frac{1}{2\pi i} \iint_{\nu \in \mathbb{C}} \frac{d\nu \wedge d\bar{\nu}}{\nu - \lambda} \\ & \times \iint_{\mu \in \mathbb{C}} d\mu \wedge d\bar{\mu} \chi(\mu, \mathbf{x}) g(\nu, \mathbf{x}) \\ & \times R(\nu, \mu) g^{-1}(\mu, \mathbf{x}) \end{aligned} \quad [7]$$

This equation can be derived using the generalized Cauchy formula. Let $f(z)$ be a smooth (not necessarily holomorphic) function in a bounded domain D in the complex plane. Then

$$\begin{aligned} f(z) = & \frac{1}{2\pi i} \oint_{\partial D} \frac{d\chi}{\chi - z} f(\chi) \\ & + \frac{1}{2\pi i} \iint_D \frac{d\chi \wedge d\bar{\chi}}{\chi - z} \frac{\partial f(\chi)}{\partial \bar{\chi}} \end{aligned} \quad [8]$$

If the kernel $g(\lambda, \mathbf{x}) R(\lambda, \mu) g^{-1}(\mu, \mathbf{x})$ is sufficiently good (e.g., it is sufficient to assume, that $(1 + |\lambda|)^{1+\epsilon} g(\lambda, \mathbf{x}) R(\lambda, \mu) g^{-1}(\mu, \mathbf{x}) (1 + |\mu|)^2$, $\epsilon > 0$, is a continuous function at both finite and infinite points), then we have a Fredholm equation (the operator on the right-hand side of [7] is compact). If it has no unit eigenvalues, eqn [7] is uniquely solvable. But, for some values of \mathbf{x} , one of the eigenvalues may become equal to 1, and it results in singularities of solutions.

If the norm of the integral operator is smaller than 1, eqn [7] is uniquely solvable. To generate solutions that are regular for all values of physical variables, it is natural to restrict the class of admissible spectral data by assuming the kernel $g(\lambda, \mathbf{x}) R(\lambda, \mu) g^{-1}(\mu, \mathbf{x})$ to be bounded in \mathbf{x} for all λ, μ . In the scalar case $n = 1$, this restriction implies:

$$\begin{aligned} R(\lambda, \mu) = & 0 \\ & \text{for all } \lambda, \mu \text{ such that } g(\lambda, \mathbf{x}) g^{-1}(\mu, \mathbf{x}) \\ & \text{is unbounded in } \mathbf{x} \end{aligned} \quad [9]$$

For specific examples like the Kadomtsev–Petviashvili-II (KP-II), direct scattering transform automatically generates spectral data satisfying [9]. In KP-II, [9] implies

$$R(\lambda, \mu) = A(\lambda) \delta(\lambda - \mu) + T(\lambda) \delta(\lambda - \bar{\mu}) \quad [10]$$

The coefficient $A(\lambda)$ can be eliminated by multiplying the wave function to an appropriate function of λ ; therefore, in standard texts, $A(\lambda) \equiv 0$.

If for every λ the kernel $R(\lambda, \mu)$ is equal to 0 everywhere except at finite number of points $\mu_1(\lambda), \dots, \mu_k(\lambda)$, one has the so-called local $\bar{\partial}$ -problem. Such kernels are rather typical.

Examples of Soliton Systems Integrable by the $\bar{\partial}$ -Problem Method

Let us discuss some important examples.

The KP-II Hierarchy

The first nontrivial equation from the KP hierarchy has the following form:

$$(u_t + 6uu_x - u_{xxx})_x = 3\alpha^2 u_{yy} \quad [11]$$

From a physical point of view, the case of real α^2 is the most interesting one. Equation [11] is called KP-I if $\alpha^2 = -1$ and KP-II if $\alpha^2 = +1$. The Lax pair for KP-II reads:

$$[L, A] = 0$$

where

$$\begin{aligned} L = & \partial_y - \partial_x^2 + u(x, y, t) \\ A = & \partial_t - 4\partial_x^3 + 6u(x, y, t)\partial_x \\ & + 3u_x(x, y, t) + 3w(x, y, t) \end{aligned} \quad [12]$$

The Cauchy problem for initial data $u(x, y, 0)$ decaying at infinity is solved by using the nonlocal Riemann problem for KP-I and local $\bar{\partial}$ -problem for KP-II. The wave function is assumed to be scalar valued ($n = 1$), and $\bar{\partial}$ -equation [4] takes the following form:

$$\frac{\partial \Psi(\lambda, x, y, t)}{\partial \bar{\lambda}} = T(\lambda) \Psi(\bar{\lambda}, x, y, t) \quad [13]$$

The wave function $\Psi(\lambda, x, y, t)$ is assumed to be regular for finite λ 's and to have the following essential singularity as $\lambda \rightarrow \infty$:

$$\Psi(\lambda, x, y, t) = \exp(\lambda x + \lambda^2 y + 4\lambda^3 t)(1 + o(1)) \quad [14]$$

Equivalently, $\eta(\lambda) \equiv 1$ and the function $g(\lambda, x, t)$ has one essential singularity at $\lambda \rightarrow \infty$,

$$g(\lambda, x, t) = \exp(\lambda x + \lambda^2 y + 4\lambda^3 t) \quad [15]$$

Higher times t_k from the KP hierarchy are incorporated into this scheme by assuming that

$$g(\lambda, t) = \exp\left(\sum_{k=1}^{\infty} \lambda^k t_k\right) \quad [16]$$

Here $x = t_1$, $y = t_2$, $t = 4t_3$.

Equation [13] was originally derived (Ablowitz *et al.* 1983) from the direct spectral transform. If the potential $u(x, y)$ is sufficiently small and $u(x, y) = O(1/(x^2 + y^2)^{1+\epsilon})$ for $x^2 + y^2 \rightarrow \infty$, then the wave function $\Psi(\lambda, x, y)$ for the L -operator [12]

$$\begin{aligned} L\Psi(\lambda, x, y) &= 0 \\ \Psi(\lambda, x, y) &= \exp(\lambda x + \lambda^2 y)[1 + o(1)] \\ &\text{for } x^2 + y^2 \rightarrow \infty \end{aligned} \quad [17]$$

can be constructed by solving the following integral equation for the pre-exponent $\chi(\lambda, x, y) = \Psi(\lambda, x, y) \exp(-\lambda x - \lambda^2 y)$:

$$\begin{aligned} \chi(\lambda, x, y) &= 1 - \iint G(\lambda, x - x', y - y') u(x, y) \\ &\quad \times \chi(\lambda, x, y) dx' dy' \end{aligned} \quad [18]$$

where the Green function $G(\lambda, x, y)$ is given by

$$G(\lambda, x, y) = \frac{1}{4\pi^2} \iint \frac{e^{i(p_x x + p_y y)}}{p_x^2 + ip_y - 2i\lambda p_x} dp_x dp_y \quad [19]$$

It is not holomorphic in λ , but

$$\frac{\partial G(\lambda, x, y)}{\partial \bar{\lambda}} = -\frac{i}{2\pi} \operatorname{sgn}(\Re \lambda) e^{-2i\Re \lambda x - 4i\Re \lambda \Im \lambda y} \quad [20]$$

The nonholomorphicity of $G(\lambda, x, y)$ results in the special nonholomorphicity of $\Psi(\lambda, x, y)$ of the form [13].

Remark We see that one function of two real variables $T(\lambda)$ is sufficient to solve the Cauchy problem in the plane. But it is also possible to construct solutions of KP-II starting from generic nonlocal kernels $R(\lambda, \mu)$ (to guarantee at least local existence of solutions, it is enough to assume that $R(\lambda, \mu)$ is small and has finite support). It looks like a paradox, but the situation is exactly the same in the linear case. In the standard Fourier method, only exponents with real momenta are used, but local solutions can be constructed as combinations of exponents with arbitrary complex momenta.

Novikov-Veselov Hierarchy and Two-Dimensional Schrödinger Operator

Equations from this hierarchy admit representation in terms of Manakov L–A–B triples,

$$\frac{\partial L}{\partial t_n} = [A_n, L] + B_n L \quad [21]$$

where

$$\begin{aligned} L &= -4\partial_z \partial_{\bar{z}} + u(z, t) \\ A_n &= 2^{2n+1} (\partial_z^{2n+1} + \partial_{\bar{z}}^{2n+1}) + \dots \end{aligned} \quad [22]$$

The order of B_n is smaller than $2n + 1$. In particular, for $n = 1$,

$$\begin{aligned} A_1 &= 8(\partial_z^3 + \partial_{\bar{z}}^3) + 2(u\partial_z + \bar{u}\partial_{\bar{z}}) \\ B_1 &= w_z + \bar{w}_{\bar{z}} \end{aligned} \quad [23]$$

$$u_t = 8\partial_z^3 u + 8\partial_{\bar{z}}^3 u + 2\partial_{\bar{z}}(uw) + 2\partial_z(u\bar{w}) \quad [24]$$

where

$$u(z, t) = \bar{u}(z, t), \quad \partial_z w(z, t) = -3\partial_{\bar{z}} u(z, t) \quad [25]$$

This hierarchy is integrated using the scattering transform at zero energy for the two-dimensional Schrödinger operator L . If Cauchy data with asymptotic

$$u(z) \rightarrow -E_0, \quad w(z) \rightarrow 0, \quad \text{for } |z| \rightarrow \infty \quad [26]$$

is considered, the scattering transform for the operator $\tilde{L} = L + E_0$ with the potential $\tilde{u}(z) = u(z) + E_0$ at fixed energy E_0 and decaying at infinity is used. In fact, the fixed-energy scattering problem is one of the basic problems of mathematical physics, and the Novikov–Veselov hierarchy can be treated as an infinite-dimensional Abel symmetry algebra for this problem. The scattering transform essentially depends on the sign of E_0 . The case $E_0 = 0$, studied by Boiti, Leon, Manna, and Pempinelli is the most complicated from the analytic point of view, and we do not discuss it now.

If $E_0 < 0$, the wave function satisfies a pure local $\bar{\partial}$ -relation:

$$\frac{\partial \Psi(\lambda, z)}{\partial \bar{\lambda}} = T(\lambda) \Psi\left(\frac{1}{\bar{\lambda}}, z\right) \quad [27]$$

with $\eta(\lambda) \equiv 1$, and

$$g(\lambda, z) = e^{(\kappa/2)(\lambda \bar{z} + z/\lambda)}, \quad \kappa^2 = -E_0 \quad [28]$$

Starting from generic spectral data $T(\lambda)$, one obtains a fixed-energy eigenfunction for a second-order operator,

$$\begin{aligned} \tilde{L}\Psi(\lambda, z) &= E_0 \Psi(\lambda, z) \\ L &= -4\partial_z \partial_{\bar{z}} + V(z) \partial_z + \tilde{u}(z) \end{aligned} \quad [29]$$

To generate pure potential operators ($V(z) \equiv 0$), it is necessary to impose additional symmetry constraints of the spectral data (see the section “Reductions on the $\bar{\partial}$ -data”).

If $E_0 > 0$, there are two types of generalized spectral data – $\bar{\partial}$ -data and nonlocal Riemann problem data. The wave function satisfies the $\bar{\partial}$ -relation:

$$\frac{\partial \Psi(\lambda, z)}{\partial \bar{\lambda}} = T(\lambda) \Psi\left(-\frac{1}{\bar{\lambda}}, z\right), \quad |\lambda| \neq 1 \quad [30]$$

and has a jump at the unit circle $|\lambda| = 1$. The boundary values $\Psi_{\pm}(\lambda, z) = \Psi(\lambda(1 \pm 0), z)$ are connected by the following relation:

$$\Psi_+(\lambda, z) = \Psi_-(\lambda, z) + \oint_{|\mu|=1} R(\lambda, \mu) \Psi_-(\mu, z) |d\mu| \quad [31]$$

$$g(\lambda, z) = e^{i(\kappa/2)(\lambda \bar{z} + z/\lambda)}, \quad \kappa^2 = E_0 \quad [32]$$

Constraints on the spectral data associated with pure potential operators were found by Novikov and Grinevich for $R(\lambda, \mu)$, and by Manakov and Grinevich for $T(\lambda)$. Existence of two different types of generalized scattering data has a very transparent physical meaning: there is a one-to-one correspondence between the classical scattering amplitude at energy E_0 and the nonlocal Riemann problem data $R(\lambda, \mu)$. The $\bar{\partial}$ -data $T(\lambda)$ can be treated as a complete set of additional parameters enumerating all potentials with a given scattering amplitude at one energy.

Davey–Stewartson-II and Ishimori-I Equations

The Davey–Stewartson-II (DS-II) equation

$$i\partial_t q + 2(\partial_z^2 + \partial_{\bar{z}}^2)q + (g + \bar{g})q = 0 \quad [33]$$

$$\partial_{\bar{z}} g = -\kappa \partial_z |q|^2 \quad [34]$$

$$q = q(z, t), \quad g = g(z, t), \quad z = x + iy \quad [35]$$

can be treated as an integrable $(2+1)$ -dimensional extension of nonlinear Schrödinger equation. The Ishimori-I equation

$$\partial_t S + S \times (\partial_x^2 S + \partial_y^2 S) + \partial_x w \partial_y S + \partial_y w \partial_x S = 0 \quad [36]$$

$$\partial_x^2 w - \partial_y^2 w + 2S(\partial_x S \times \partial_y S) = 0 \quad [37]$$

$$S = S(x, y, t), \quad S = (S_1, S_2, S_3), \quad S^2 = 1 \quad [38]$$

is an integrable $(2+1)$ -dimensional extension of the Heisenberg magnetic equation. Both systems are

integrated by using the following zero-curvature representation:

$$\begin{pmatrix} \partial_{\bar{z}} & 0 \\ 0 & \partial_z \end{pmatrix} \Psi = \frac{1}{2} \begin{pmatrix} 0 & q(z, t) \\ \kappa q(z, t) & 0 \end{pmatrix} \Psi \quad [39]$$

$$\partial_t \Psi = \begin{pmatrix} 2i\partial_z^2 + ig & iq_{\bar{z}} - iq\partial_{\bar{z}} \\ -i\kappa q_{\bar{z}} + i\kappa q\partial_z & -2i\partial_{\bar{z}}^2 - ig \end{pmatrix} \Psi \quad [40]$$

The wave function satisfies the following “scattering” equation:

$$\begin{pmatrix} \partial_k & 0 \\ 0 & \partial_k \end{pmatrix} \Psi^T = \begin{pmatrix} 0 & \kappa \bar{b}(k) \\ b(k) & 0 \end{pmatrix} \Psi^T \quad [41]$$

Here Ψ^T denotes the transposed matrix. Let us point out the amazing symmetry between the direct and inverse transforms.

Discrete Systems

In the examples discussed above, continuous variables are “encoded” in essential singularities of $g(\lambda, x)$. Discrete variables correspond to orders of zeros and poles. For example, assuming that the function $g(\lambda, t)$ in the KP integration scheme depends on extra continuous variables $t_{-1}, t_{-2}, \dots, t_{-n}, \dots$ and discrete variable $t_0 = n$,

$$g(\lambda, t) = \lambda^{t_0} \exp\left(\sum_{k \neq 0} \lambda^k t_k\right) \quad [42]$$

one obtains solutions of the so-called two-dimensional Toda–KP hierarchy.

Assume that we have a nonlocal $\bar{\partial}$ -problem for a scalar function with $\eta \equiv 1$ and

$$g(\lambda, n_1, \dots, n_k) = \prod_{j=1}^k \left(\frac{\lambda - P_k}{\lambda - Q_k} \right)^{n_k} \quad [43]$$

The wave function defines a map $\mathbb{Z}^k \rightarrow \mathbb{C}^N$,

$$(n_1, \dots, n_k) \rightarrow (\Psi(\lambda_1, n_1, \dots, n_k), \dots, \Psi(\lambda_N, n_1, \dots, n_k)) \quad [44]$$

where $\lambda_1, \dots, \lambda_N$ are some points in \mathbb{C} . This construction generates the so-called quadrilateral lattices (each two-dimensional face is planar).

Multidimensional Problems

The $\bar{\partial}$ -approach can also be applied to multidimensional inverse-scattering problems, but typically the scattering data are overdetermined and satisfy additional nonlinear compatibility conditions. For

example, the Faddeev wave functions for the n -dimensional stationary Schrödinger operator

$$(-\partial_{x_1}^2 - \dots - \partial_{x_n}^2 + u(x))\Psi(k, x) = (k \cdot k)\Psi(k, x) \quad [45]$$

$$\Psi(k, x) = e^{ik \cdot x}(1 + o(1)) \quad [46]$$

in the nonphysical domain $k_I \neq 0$ (k_R and k_I denote the real and imaginary parts of k , respectively) satisfy the following $\bar{\partial}$ -equation:

$$\frac{\partial \Psi(k, x)}{\partial \bar{k}_j} = -2\pi \int_{\xi \in \mathbb{R}^n} \xi_j h(k, k_R + \xi) \Psi(k + \xi, x) \times \delta(\xi \cdot \xi + 2k \cdot \xi) d\xi_1 \dots d\xi_n \quad [47]$$

The characterization of admissible spectral data $h(k, l), k \in \mathbb{C}^n, l \in \mathbb{R}^n$ is based on the following compatibility equation:

$$\begin{aligned} \frac{\partial h(k, l)}{\partial \bar{k}_j} + \frac{1}{2} \frac{\partial h(k, l)}{\partial l_j} \\ = -2\pi \int_{\xi \in \mathbb{R}^n} \xi_j h(k, k_R + \xi) h(k + \xi, l) \\ \times \delta(\xi \cdot \xi + 2k \cdot \xi) d\xi_1 \dots d\xi_n \end{aligned} \quad [48]$$

More details can be found in Novikov and Henkin (1987).

Reductions on the $\bar{\partial}$ -Data

The most generic $\bar{\partial}$ -data usually result in solutions from wrong functional class (they may, e.g., be complex or singular), or extra constraints on the auxiliary linear operators are necessary to obtain solutions of the zero-curvature representation. For example, to obtain real KP-II solutions using the local $\bar{\partial}$ -problem [13], the following reduction on the $\bar{\partial}$ -data should be implied:

$$T(\bar{\lambda}) = -\bar{T}(\lambda) \quad [49]$$

It can be easily derived from the direct transform. But it is not always the case. For example, the selection of pure potential two-dimensional Schrödinger operators originally was not so evident. To formulate the answer, it is convenient to introduce a new function $b(\lambda), T(\lambda) = b(\lambda)\pi \operatorname{sgn}(\lambda\bar{\lambda} - 1)/\bar{\lambda}$.

For $E_0 < 0$, the following constraints select real potential operators:

$$b\left(-\frac{1}{\bar{\lambda}}\right) = b(\lambda), \quad b\left(\frac{1}{\bar{\lambda}}\right) = \bar{b}(\lambda) \quad [50]$$

In some situations, the problem of finding appropriate reductions is the most difficult part of the integration procedure. It is true not only for the

$\bar{\partial}$ -approach, but also for other techniques including the finite-gap method. For example, the inverse-spectral transform for the two-dimensional Schrödinger operator was first developed for finite-gap (quasiperiodic) potentials and only later for the decaying ones. For operators with finite gap at one energy the first-order terms were constructed by Dubrovin, Krichever, and Novikov in 1976, but only in 1984 the potentiality reduction was found by Novikov and Veselov.

Nonsingular Solutions

As mentioned above, one can construct regular solutions by choosing sufficiently small (in an appropriate norm) scattering data. But for some special systems the regularity follows automatically from reality reductions. For example, for arbitrary large $\bar{\partial}$ -data, real KP-II solutions constructed by the local $\bar{\partial}$ -problem [13] with reduction [49] are regular. The proof is based on the theory of generalized analytic functions (in the Vekua sense). Another example is the two-dimensional Schrödinger operator at a fixed negative energy $E_0 < 0$. The potentiality and reality constraints imply that the potential is nonsingular for arbitrary large $T(\lambda)$. But, unfortunately, the $\bar{\partial}$ -problem with regular data covers only a part of the space of potentials. In fact, each such operator possesses a strictly positive real eigenfunction at the level E_0 , exponentially growing in all directions (it also follows from the generalized analytic functions theory). Existence of such function implies that the whole discrete spectrum is located above the energy E_0 , and it gives a restriction on the potential. (For more details, see the review by Grinevich (2000).)

Some Explicit Solutions

The generic $\bar{\partial}$ -problem results in potentials that could not be expressed in terms of elementary or standard special functions. But for degenerate kernels, a solution of the inverse-spectral problem can be written explicitly. For example, if

$$R(\lambda, \mu) = \sum_{k=1}^n r_k(\lambda) s_k(\mu) \quad [51]$$

the wave function and solutions can be expressed in quadratures.

In particular, if all $r_k(\lambda)$ and $s_k(\mu)$ are δ -functions, $r_k(\lambda) = R_k \delta(\lambda - \lambda_k)$ and $s_k(\mu) = S_k \delta(\mu - \mu_k)$, the wave function is rational in λ and can be expressed as a rational combination of exponents of x_k . If for some k and l , $\lambda_k = \mu_l$, this procedure needs some

regularization. For example, it is possible to assume, that $\delta(\lambda - \lambda_0)/(\lambda - \lambda_0) = 0$.

If for all k , $\lambda_k = \mu_k$, the $\bar{\partial}$ -problem generates rational in x solutions (lumps). It is possible to show that, the Novikov–Veselov real rational solitons for $E_0 > 0$ are always nonsingular, decay at ∞ as $1/(x^2 + y^2)$, and the potential $u(z)$ has zero scattering in all directions for the waves with energy E_0 .

The $\bar{\partial}$ -Problem on Riemann Surfaces

In all examples discussed above, the spectral variable is defined in a Riemann sphere. It is natural to generalize it by considering wave functions depending on a spectral parameter defined on a Riemann surface of higher genus. Spectral transforms of such type arise in the theory of localized perturbation of periodic solutions. Assume that the KP-II potential $u(x, y)$ has the form

$$u(x, y) = u_0(x, y) + u_1(x, y) \quad [52]$$

where $u_0(x, y)$ is a real nonsingular finite-gap potential and $u_1(x, y)$ decays sufficiently fast at infinity. Denote by $\Psi_0(\gamma, x, y)$ the wave function of the operator $L_0 = \partial_y - \partial_x^2 + u_0(x, y)$, where $\gamma \in \Gamma$, the spectral curve Γ is a compact Riemann surface of genus g with a distinguished point ∞ . In addition to essential singularity at the point ∞ , the wave function $\Psi_0(\gamma, x, y)$ has g simple poles at points $\gamma_1, \dots, \gamma_g$ and is holomorphic in γ outside these singular points. For a real nonsingular potential, Γ is an M -curve, that is, there exists an antiholomorphic involution $\tau: \Gamma \rightarrow \Gamma, \tau\infty = \infty$, the set of fixed points form $g + 1$ ovals $a_0, \dots, a_g, \infty \in a_0, \gamma_k \in a_k$. The wave function $\Psi(\gamma, x, y)$ of the perturbed operator $L = \partial_y - \partial_x^2 + u(x, y)$ is defined at the same spectral curve Γ , but it is not holomorphic any more. It has the following properties:

1. At the point ∞ , the wave function $\Psi(\gamma, x, y)$ has an essential singularity: $\Psi(\gamma, x, y) = \Psi_0(\gamma, x, y)(1 + o(1))$.
2. In the neighborhoods of the points γ_k , $\Psi(\gamma, x, y)$ can be written as a product of a continuous function by a simple pole at γ_k .
3. The wave function $\Psi(\gamma, x, y)$ satisfies the $\bar{\partial}$ equation

$$\frac{\partial \Psi(\gamma, x, y, t)}{\partial \bar{\gamma}} d\bar{\gamma} = T(\gamma) \Psi(\tau\gamma, x, y, t) \quad [53]$$

where the $(0, 1)$ -form $T(\gamma) = t(\gamma)d\bar{\gamma}$ is regular outside the divisor points γ_k and in the neighborhood of γ_k it possible to define local coordinate such that $t(\gamma) = \text{sgn}(\Im \gamma) t_1(\gamma)(\gamma - \gamma_k)/(\gamma - \gamma_k), t_1(\gamma)$ is regular.

A solution of the inverse problem can be obtained by using appropriate analogs of Cauchy kernels on Riemann surfaces.

Quasiclassical Limit

The systems integrable by the $\bar{\partial}$ -method usually describe integrable systems with high-order derivatives. It is well known that by applying some limiting procedures to integrable systems one can construct new completely integrable equations, but integration methods for these equations are based on completely different analytic tools. One of most important examples is the theory of dispersionless hierarchies. The limiting procedure for the $\bar{\partial}$ -problem (quasiclassical $\bar{\partial}$ -problem) was developed by Konopelchenko and collaborators. In the KP case, the quasiclassical limit of the wave function $\Psi(\lambda, t)$ is assumed to have the following form:

$$\Psi\left(\lambda, \frac{t}{\epsilon}\right) = \hat{\chi}(\lambda, t, \epsilon) \exp\left(\frac{S(\lambda, t)}{\epsilon}\right) \quad [54]$$

It is possible to show that the function $S(\lambda, t)$ satisfies a Beltrami-type equation:

$$\frac{S(\lambda, t)}{\partial \bar{\lambda}} = W\left(\lambda, \frac{S(\lambda, t)}{\partial \lambda}\right) \quad [55]$$

which is treated as a dispersionless limit of [13]. Higher-order corrections were also discussed in the literature (see Konopelchenko and Moro (2003)).

See also: Boundary-Value Problems for Integrable Equations; Integrable Systems and Algebraic Geometry; Integrable Systems and the Inverse Scattering Method; Integrable Systems: Overview; Integrable Systems and Discrete Geometry; Riemann–Hilbert Methods in Integrable Systems.

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Derived Categories

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Introduction

In this article we shall briefly outline derived categories and their relevance for physics. Derived categories (and their enhancements) classify off-shell states in a two-dimensional topological field theory on Riemann surfaces with boundary known as the open-string B model. We briefly review pertinent aspects of that topological field theory and its relation to derived categories, the Bondal–Kapranov enhancement and its relation to the open-string B model, as well as B model twists of two-dimensional theories known as Landau–Ginzburg models, and how information concerning stability of D-branes is encoded in this language. We concentrate on more physical aspects of derived categories; for a very readable short review concentrating on the mathematics, see, for example, Thomas (2000).

Sheaves and Derived Categories in the Open-String B Model

Derived categories are mathematical constructions which are believed to be related to D-branes in the open-string B model. We shall begin by briefly reviewing the B model, as well as D-branes.

The A and B models are two-dimensional topological field theories, closely related to nonlinear sigma models, which are supersymmetrizations of theories summing over maps from a Riemann surface (the world sheet of the string) into some “target space” X . In both the A and B models, one considers only certain special correlation functions, involving correlators closed under the action of a nilpotent scalar operator known as the “BRST operator,” Q , which is part of the original supersymmetry transformations. In considering the pertinent correlation functions, only certain types of maps contribute. The A model has the properties of

being invariant under complex structure deformations of the target space X , and its pertinent correlation functions are computed by summing over holomorphic maps into the target X . The A model will not be relevant for us here. The B model has the properties of being invariant under Kähler moduli of the target X , and its pertinent correlation functions are computed by summing over constant maps into the target X . In the closed-string B model, the states of the theory are counted by the cohomology groups $H^*(X, \Lambda^*TX)$, where X is constrained to be Calabi–Yau. The BRST operator in the B model Q can be identified with $\bar{\partial}$ for many purposes. The open-string B model is the same topological field theory, but now defined on a Riemann surface with boundaries. As with all open-string theories, we specify boundary conditions on the fields, which force the ends of the string to live on some submanifold of the target, and we associate to the boundaries degrees of freedom (known as the Chan–Paton factors) which describe a (possibly twisted) vector bundle over the submanifold. In the case of the B model, the submanifold is a complex submanifold, and the vector bundle is forced to be a holomorphic vector bundle over that submanifold.

To lowest order, that combination of a submanifold S of X together with a (possibly twisted) holomorphic vector submanifold, is a “D-brane” in the open-string B model. We shall denote the twisted bundle by $\mathcal{E} \otimes \sqrt{K_S}$, where K_S is the canonical bundle of S , and the $\sqrt{K_S}$ factor is an explicit incorporation of something known as the Freed–Witten anomaly. Now, if $i: S \hookrightarrow X$ is the inclusion map, then to this D-brane we can associate a sheaf $i_*\mathcal{E}$.

Technically, a sheaf is defined by associating sets, or modules, or rings, to each open set on the underlying space, together with restriction maps saying how data associated to larger open sets restricts to smaller open sets, obeying the obvious consistency conditions, together with some gluing conditions that say how local sections can be patched back together. A vector bundle defines a

sheaf by associating to any open set sections of the bundle over that open set. Sheaves of the form “ $i_*\mathcal{E}$ ” look like, intuitively, vector bundles over submanifolds, with vanishing fibers off the submanifold. A more detailed discussion of sheaves is beyond the scope of this article; see instead, for example, Sharpe (2003).

To “associate a sheaf” means finding a sheaf such that physical properties of the D-brane system are well modeled by mathematics of the sheaf. (In particular, the physical definition of D-brane has, on the face of it, nothing at all to do with the mathematical definition of a sheaf, so one cannot directly argue that they are the same, but one can still use one to give a mathematical model of the other.) For example, the spectrum of open-string states in the B model stretched between two D-branes, associated to sheaves $i_*\mathcal{E}$ and $j_*\mathcal{F}$, turn out to be calculated by a cohomology group known as $\text{Ext}_X^*(i_*\mathcal{E}, j_*\mathcal{F})$.

There are many more sheaves not of the form $i_*\mathcal{E}$, that is, that do not look like vector bundles over submanifolds. It is not known in general whether they also correspond to (on-shell) D-branes, but in some special cases the answer has been worked out. For example, structure sheaves of nonreduced schemes turn out to correspond to D-branes with nonzero nilpotent Higgs vevs.

For a set of ordinary D-branes, the description above suffices. However, more generally one would like to describe collections of D-branes and anti-D-branes, and tachyons. An anti-D-brane has all the same physical properties as an ordinary D-brane, modulo the fact that they try to annihilate each other. The open-string spectrum between coincident D-branes and anti-D-branes contains tachyons. One can give an (off-shell) vacuum expectation value to such tachyons, and then the unstable brane–antibrane–tachyon system will evolve to some other, usually simpler, configuration. For example, given a single D-brane wrapped on a curve, with trivial line bundle, and an anti-D-brane wrapped on the same curve, with line bundle $\mathcal{O}(-1)$, and a nonzero tachyon $\mathcal{O}(-1) \rightarrow \mathcal{O}$, then one expects that the system will dynamically evolve to a smaller D-brane sitting at a point on the curve.

Now, one would like to find some mathematics that describes such systems, and gives information about the endpoints of their evolution. Technically, one would like to classify universality classes of world-sheet boundary renormalization group flow.

It has been conjectured that derived categories of sheaves provide such a classification. To properly explain derived categories is well beyond the scope

of this article (see instead the “Further reading” section at the end), but we shall give a short outline below.

Mathematically, derived categories of sheaves concern complexes of sheaves, that is, sets of sheaves \mathcal{E}_i together with maps $d_i: \mathcal{E}_i \rightarrow \mathcal{E}_{i+1}$

$$\cdots \longrightarrow \mathcal{E}_i \xrightarrow{d_i} \mathcal{E}_{i+1} \xrightarrow{d_{i+1}} \mathcal{E}_{i+2} \xrightarrow{d_{i+2}} \cdots$$

such that $d_{i+1} \circ d_i = 0$. A category is defined by a collection of “objects” together with maps between the objects, known as morphisms. In a derived category of coherent sheaves, the objects are complexes of sheaves, and the maps are equivalence classes of maps between complexes.

Physically, if the complex consists of locally free sheaves (equivalently, vector bundles), then we can associate a brane/antibrane/tachyon system, by identifying the \mathcal{E}_i for i even, say, with D-branes, and the \mathcal{E}_i for i odd with anti-D-branes. If the \mathcal{E}_i are all locally free sheaves, then there are tachyons between the branes and antibranes, and we can identify the d_i ’s with those tachyons. In the open-string world-sheet theory, giving a tachyon a vacuum expectation value modifies the BRST operator Q , and a necessary condition for the new theory to still be a topological field theory is that $Q^2 = 0$, a condition which turns out to imply that $d_{i+1} \circ d_i = 0$.

To re-create the structure of a derived category, we need to impose some equivalence relations. To see what sorts of equivalence relations one would like to impose, note the following. Physically, we would like to identify, for example, a configuration consisting of a brane, an antibrane, and a tachyon, which we can describe as a complex

$$\mathcal{O}(-D) \longrightarrow \mathcal{O}$$

with a one-element complex

$$\mathcal{O}_D$$

corresponding to the D-brane which we believe is the endpoint of the evolution of the brane/antibrane configuration.

One natural mathematical way to create identifications of this form is to identify complexes that differ by “quasi-isomorphisms,” meaning, a set of maps $(f^n: C^n \rightarrow D^n)$ compatible with d ’s, and inducing an isomorphism $\tilde{f}^n: H^n(C) \cong H^n(D)$ on the cohomologies of the complexes. In particular, in the example above, there is a natural set of maps

$$\begin{array}{ccc} \mathcal{O}(-D) & \longrightarrow & \mathcal{O} \\ \downarrow & & \downarrow \\ 0 & \longrightarrow & \mathcal{O}_D \end{array}$$

that define a quasi-isomorphism. More generally, in homological algebra, one typically does computations by replacing ordinary objects with projective or injective resolutions, that is, complexes with special properties, in which the desired computation becomes trivial, and defining the result for the original object to be the same as the result for the resolution. To formalize this procedure, one would like a mathematical setup in which objects and their projective and injective resolutions are isomorphic.

However, to define an equivalence relation, one usually needs an isomorphism, and the quasi-isomorphisms above are not, in general, isomorphisms. Creating an equivalence from nonisomorphisms, to resolve this problem, can be done through a process known as “localization” (generalizing the notion of localization in commutative algebra). The resulting equivalence relations on maps between complexes define the derived category.

The derived category is a category whose objects are complexes, and whose morphisms $C \rightarrow D$ are equivalence classes of pairs (s, t) where $s: G \rightarrow C$ is a quasi-isomorphism between C and another complex G , and $t: G \rightarrow D$ is a map of complexes. We take two such pairs $(s, t), (s', t')$ to be equivalent if there exists another pair (r, h) between the auxiliary complexes G, G' , making the obvious diagram commute. This is, in a nutshell, what is meant by localization, and by working with such equivalence classes, this allows us to formally invert maps that are otherwise noninvertible. (We encourage the reader to consult the “Further reading” section for more details.)

Mathematically, this technology gives a very elegant way to rethink, for example, homological algebra. There is a notion of a derived functor, a special kind of functor between derived categories, and notions from homological algebra such as Ext and Tor can be re-expressed as cohomologies of the image complexes under the action of a derived functor, thus replacing cohomologies with complexes.

Physically, looking back at the physical realization of complexes, we see a basic problem: different representatives of (isomorphic) objects in the derived category are described by very different physical theories. For example, the sheaf \mathcal{O}_D corresponds to a single D-brane, defined by a two-dimensional boundary conformal field theory (CFT), whereas the brane/antibrane/tachyon collection $\mathcal{O}(-D) \rightarrow \mathcal{O}$ is defined by a massive nonconformal two-dimensional theory. These are very different physical theories. If we want “localization on quasi-isomorphisms” to happen in physics, we have to explain which properties of the physical theories we

are interested in, because clearly the entire physical theories are not and cannot be isomorphic.

Although the entire physical theories are not isomorphic, we can hope that under renormalization group flow, the theories will become isomorphic. That is certainly the physical content of the statement that the brane/antibrane system $\mathcal{O}(-D) \rightarrow \mathcal{O}$ should describe the D-brane corresponding to \mathcal{O}_D – after world-sheet boundary renormalization group flow, the nonconformal two-dimensional theory describing the brane/antibrane system becomes a CFT describing a single D-brane.

More globally, this is the general prescription for finding physical meanings of many categories: we can associate physical theories to particular types of representatives of isomorphism classes of objects, and then although distinct representatives of the same object may give rise to very different physical theories, those physical theories at least lie in the same universality class of world-sheet renormalization group flow. In other words, (equivalence classes of) objects are in one-to-one correspondence with universality classes of physical theories.

Showing such a statement directly is usually not possible – it is usually technically impractical to follow renormalization group flow explicitly. There is no symmetry reason or other basic physics reason why renormalization group flow must respect quasi-isomorphism. The strongest constraint that is clearly applied by physics is that renormalization group flow must preserve D-brane charges (Chern characters, or more properly, K -theory), but objects in a derived category contain much more information than that.

However, indirect tests can be performed, and because many indirect tests are satisfied, the result is generally believed.

The reader might ask why it is not more efficient to just work with the cohomology complexes $H^*(C)$ themselves, rather than the original complexes. One reason is that the original complexes contain more information than the cohomology – passing to cohomology loses information. For example, there exist examples of complexes that have the same cohomology, yet are not quasi-isomorphic, and so are not identified within the derived category, and so physically are believed to lie in different universality classes of boundary renormalization group flow.

Another motivation for relating physics to derived categories is Kontsevich’s approach to mirror symmetry. Mirror symmetry relates pairs of Calabi–Yau manifolds, of the same dimension, in a fashion such that easy classical computations in one Calabi–Yau

are mapped to difficult “quantum” computations involving sums over holomorphic curves in the other Calabi–Yau. Because of this property, mirror symmetry has proved a fertile ground for algebraic geometers to study. Kontsevich proposed that mirror symmetry should be understood as a relation between derived categories of coherent sheaves on one Calabi–Yau and derived Fukaya categories on the other Calabi–Yau. At the time he made this proposal, no one had any idea how either could be realized in physics, but since that time, physicists have come to believe that Kontsevich was secretly talking about D-branes in the A and B models.

Bondal–Kapranov Enhancements

Mathematically derived categories are not quite as ideal as one would like. For example, the cone construction used in triangulated categories does not behave functorially – the cone depends upon the representative of the equivalence class defining an object in a derived category, and not just the object itself.

Physically, our discussion of brane/antibrane systems was not the most general possible. One can give vacuum expectation values to more general vertex operators, not just the tachyons.

Curiously, these two issues solve each other. By incorporating a more general class of boundary vertex operators, one realizes a more general mathematical structure, due to Bondal and Kapranov, which repairs many of the technical deficiencies of ordinary derived categories. Ordinary complexes are replaced by generalized complexes in which arrows can map between non-neighboring elements of the complex. Schematically, the BRST operator is deformed by boundary vacuum expectation values to the form

$$Q = \bar{\partial} + \sum_a \phi_a$$

and demanding that the BRST operator square to zero implies that

$$\sum_a \bar{\partial} \phi_a + \sum_{a,b} \phi_b \circ \phi_a = 0$$

which is the same as the condition for a generalized complex. Note that for ordinary complexes, the condition above factors into

$$\begin{aligned} \bar{\partial} \phi_n &= 0 \\ \phi_{n+1} \circ \phi_n &= 0 \end{aligned}$$

which yields an ordinary complex of sheaves (Figure 1).

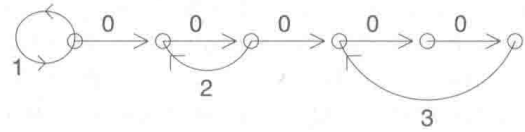


Figure 1 1. Example of generalized complex. Each arrow is labeled by the degree of the corresponding vertex operator.

Landau–Ginzburg Models

So far we have described how derived categories are relevant to geometric compactifications, that is, sigma models on Calabi–Yau manifolds. However, there are also “nongeometric” theories – CFTs that do not come from sigma models on manifolds, of which Landau–Ginzburg models and their orbifolds are prominent examples. Landau–Ginzburg models can also be twisted into topological field theories, and the B-type topological twist of (an orbifold of) a Landau–Ginzburg model is believed to be isomorphic, as a topological field theory, to the B model obtained from a nonlinear sigma model, of the form we outlined earlier. Landau–Ginzburg models have a very different form than nonlinear sigma models, and so sometimes there can be practical computational advantages to working with one rather than the other.

A Landau–Ginzburg model is an ungauged sigma model with a nonzero superpotential (a holomorphic function over the target space that defines a bosonic potential and Yukawa couplings). (In “typical” cases, the target space is a vector space.) Because of the superpotential, a Landau–Ginzburg model is a massive theory – not itself a CFT, but many Landau–Ginzburg models are believed to flow to CFTs under the renormalization group.

In formulating open strings based on Landau–Ginzburg models, naive attempts fail because of something known as the Warner problem: if the superpotential is nonzero, then the obvious ways to try to define the theory on a Riemann surface with boundary have the undesirable property that the supersymmetry transformations only close up to a nonzero boundary term, proportional to derivatives of the superpotential. In order to find a description of open strings in which the supersymmetry transformations close, one must take a very nonobvious formulation of the boundary data. Specifically, to solve the Warner problem, one is led to work with pairs of matrices whose product is proportional to the superpotential.

This method of solving the Warner problem is known as matrix factorization, and D-branes in this theory are defined by the factorization chosen, that is, the choice of pairs of matrices. In simple cases, we can be more explicit as follows. Choose a set of

polynomials F_α, G_α such that the Landau–Ginzburg superpotential W is given by

$$W = \sum_{\alpha} F_{\alpha} G_{\alpha} + \text{constant}.$$

The F_{α} and G_{α} are used to define the boundary action – the F ’s appear as part of the boundary superpotential and the G ’s appear as part of the supersymmetry transformations of boundary fermi multiplets. The F_{α} and G_{α} , that is, the factorization of W , determine the D-brane in the Landau–Ginzburg theory. We can also think of having a pair of holomorphic vector bundles $\mathcal{E}_1, \mathcal{E}_2$ of the same rank, and interpret F and G as holomorphic sections of $\mathcal{E}_1^{\vee} \otimes \mathcal{E}_2$ and $\mathcal{E}_2^{\vee} \otimes \mathcal{E}_1$, respectively, obeying $FG \propto W \cdot \text{Id}$ and $GF \propto W \cdot \text{Id}$, up to additive constants.

Although a Landau–Ginzburg model is not the same thing as a sigma model on a Calabi–Yau, orbifolds of Landau–Ginzburg models are often on the same Kähler moduli space. Perhaps, the most famous example of this relates sigma models on quintic hypersurfaces in P^4 to a Z_5 orbifold of a Landau–Ginzburg model over C^5 with five chiral superfields x_1, x_2, x_3, x_4, x_5 , and a superpotential of the form

$$W = x_1^5 + x_2^5 + x_3^5 + x_4^5 + x_5^5 \\ + \psi x_1 x_2 x_3 x_4 x_5$$

for ψ a complex number, corresponding to the equation of the degree-5 hypersurface in P^4 . The (complexified) Kähler moduli space in this example is a P^1 , with the sigma model on the quintic at one pole, the zero-volume limit of the sigma model along the equator, and the Landau–Ginzburg orbifold at the opposite pole.

Since the closed-string topological B model is independent of Kähler moduli, and the sigma model on the quintic and the Landau–Ginzburg orbifold above lie on the same Kähler moduli space, one would expect them both to have the same spectrum of D-branes, and indeed this is believed to be true.

Pi-Stability

So far we have discussed D-branes in the topological B model, a topological twist of a physical sigma model. If we untwist back to a physical sigma model, then the stability of those D-branes becomes an issue.

To begin to understand what we mean by stability in this context, consider a set of N D-branes wrapped on, say, a K3 surface, at large radius (so that world-sheet instanton corrections are small).

On the world volume of the D-branes, we have a rank- N vector bundle, and in the physical theory on that world volume we have a consistency condition for supersymmetric vacua, that the vector bundle be “Mumford–Takemoto stable.” To understand what is meant by this condition on a Kähler manifold, let ω denote the Kähler form, and define the “slope” μ of a vector bundle \mathcal{E} on a manifold X of complex dimension n to be given by

$$\mu(\mathcal{E}) = \frac{\int_X \omega^{n-1} \wedge c_1(\mathcal{E})}{\text{rank } \mathcal{E}}$$

where ω is the Kähler form. Then, we say that \mathcal{E} is (semi-)stable if for all subsheaves \mathcal{F} satisfying certain consistency conditions, $\mu(\mathcal{F})(\leq) < \mu(\mathcal{E})$.

Since the slope of a bundle depends upon the Kähler form, whether a given bundle is Mumford–Takemoto stable depends upon the metric. In general, on a Kähler manifold, the Kähler cone breaks up into subcones, with a different moduli space of (stable) holomorphic vector bundles in each subcone.

This is a mathematical notion of stability, but it also corresponds to physical stability, at least in a regime in which quantum corrections are small. If a given bundle is only stable in a proper subset of the Kähler cone, then when it reaches the boundary of the subcone in which it is stable, the gauge field configuration that satisfies the Donaldson–Uhlenbeck–Yau partial differential equation splits into a sum of two separate bundles. In a heterotic string compactification, this leads to a low-energy enhanced $U(1)$ gauge symmetry and D-terms which realize the change in moduli space. In D-branes, this means the formerly bound state of D-branes (described by an irreducible holomorphic vector bundle) becomes only marginally bound; a decay becomes possible.

Pi-stability is a proposal for generalizing the considerations above to D-branes no longer wrapping the entire Calabi–Yau, and including quantum corrections.

In order to define pi-stability, we must first introduce a notion of grading φ of a D-brane. Specifically, for a D-brane wrapped on the entire Calabi–Yau X with holomorphic vector bundle \mathcal{E} , the grading is defined as the mirror to the expression $\int_X \text{ch}(\mathcal{E}) \wedge \Pi$, where Π encodes the periods. Close to the large-radius limit, this has the form:

$$\varphi(\mathcal{E}) = \frac{1}{\pi} \text{Im} \log \int_X \exp(B + i\omega) \wedge \text{ch}(\mathcal{E}) \\ \times \wedge \sqrt{\text{td}(TX)} + \dots$$

where B is a 2-form, the “B field.” As defined φ is clearly S^1 -valued; however, we must choose a

particular sheet of the log Riemann surface, to obtain an R -valued function.

This notion of grading of D-branes is an ansatz, introduced as part of the definition of pi-stability. Physically, it is believed that the difference in grading between two D-branes corresponds to the fractional charge of the boundary-condition-changing vacuum between the two D-branes, though we know of no convincing first-principles derivation of that statement. In particular, unlike closed-string computations, the degree of the Ext group element corresponding to a particular boundary R -sector state is not always the same as the $U(1)_R$ charge – for example, it is often determined by the $U(1)_R$ charge minus the charge of the vacuum. The grading gives us the mathematical significance of that vacuum charge. This mismatch between Ext degrees and $U(1)_R$ charges is necessary for the grading to make sense: Ext group degrees are integral, after all, yet we want the grading to be able to vary continuously, so the grading had better not be the same as an Ext group degree.

Given an R -valued function from a particular definition of log in the definition of φ above, the statement of pi-stability is then that for all subsheaves \mathcal{F} , as in the statement of Mumford–Takemoto stability,

$$\varphi(\mathcal{F}) \leq \varphi(\mathcal{E})$$

Before trying to understand the physical meaning of φ , or the extension of these ideas to derived categories, let us try to confirm that Mumford–Takemoto stability emerges as a limit of pi-stability.

For simplicity, suppose that X is a Calabi–Yau 3-fold. Then, for large Kähler form ω , we can expand $\varphi(\mathcal{E})$ as,

$$\begin{aligned} \varphi(\mathcal{E}) \approx & \frac{1}{\pi} \operatorname{Im} \log \left[-\frac{i}{3!} \int_X \omega^3(\operatorname{rk} \mathcal{E}) \right] \\ & + \frac{3 \int_X \omega^2 \wedge c_1(\mathcal{E})}{\pi \int_X \omega^3(\operatorname{rk} \mathcal{E})} + \dots \end{aligned}$$

Thus, we see that to leading order in the Kähler form ω , $\varphi(\mathcal{F}) \leq \varphi(\mathcal{E})$ if and only if

$$\frac{\int_X \omega^2 \wedge c_1(\mathcal{F})}{\operatorname{rk} \mathcal{F}} \leq \frac{\int_X \omega^2 \wedge c_1(\mathcal{E})}{\operatorname{rk} \mathcal{E}}$$

which is precisely the statement of Mumford–Takemoto stability on a 3-fold X .

One can define a notion of (classical) stability for more general sheaves, but what one wants is to apply pi-stability to derived categories, not just sheaves.

However, there is a technical problem that limits such an extension. Specifically, in a derived category, there is no meaningful notion of “subobject.” Thus, a notion of stability formulated in terms of subobjects cannot be immediately applied to derived categories. There are two (equivalent) workarounds to this issue that have been discussed in the math and physics literatures, which can be briefly summarized as follows:

1. One workaround involves picking a subcategory of the derived category that does allow you to make sense of subobjects. Such a structure is known, loosely, as a “T-structure,” and so one can imagine formulating stability by first picking a T-structure, then specifying a slope function on the elements of the subcategory picked out by the subcategory.
2. Another (equivalent) workaround is to work with a notion of “relative stability.” Instead of speaking about whether a D-brane is stable against decay into any other object, one only speaks about whether it is stable against decay into pairs of specified objects.

In this fashion, one can make sense of pi-stability for derived categories.

See also: Fourier–Mukai Transform in String Theory; Mirror Symmetry: A Geometric Survey; Spectral Sequences; Superstring Theories; Topological Quantum Field Theory: Overview.

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Determinantal Random Fields

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Introduction

The theory of random point fields has its origins in such diverse areas of science as life tables, particle physics, population processes, and communication engineering. A standard reference to the subject is the monograph by Daley and Vere-Jones (1988).

This article is concerned with a special class of random point fields, introduced by Macchi in the mid-1970s. The model that Macchi considered describes the statistical distribution of a fermion system in thermal equilibrium. Macchi proposed to call the new class of random point processes the fermion random point processes. The characteristic property of this family of random point processes is the condition that k -point correlation functions have the form of determinants built from a correlation kernel. This implies that the particles obey the Pauli exclusion principle. Until the mid-1990s, fermion random point processes attracted only a limited interest in mathematics and physics communities, with the exception of two important works by Spohn (1987) and Costin-Lebowitz (1995). This situation changed dramatically at the end of the last century, as the subject greatly benefited from the newly discovered connections to random matrix theory, representation theory, random growth models, combinatorics, and number theory. Things are rapidly developing at the moment. Even the terminology has not yet set in stone. Many experts currently use the term “determinantal random point fields” instead of “fermion random point fields.” We follow this trend in our article.

This article is intended as a short introduction to the subject. The next section builds a mathematical framework and gives a formal mathematical definition of the determinantal random point fields. Then we discuss examples of determinantal random point fields from quantum mechanics, random matrix theory, random growth models, combinatorics, and representation theory. This is followed by a discussion of the ergodic properties of translation-invariant determinantal random point fields. We discuss the Gibbsian property of determinantal random point fields. Central-limit theorem type results for the counting functions and similar linear statistics are also discussed. The final section is devoted to some generalizations of determinantal point fields, namely immanantal and Pfaffian random point fields.

Mathematical Framework

We start by building a standard mathematical framework for the theory of random point processes. Let E be a one-particle space and X a space of finite or countable configurations of particles in E . In general, E can be a separable Hausdorff space. However, for our purposes it suffices to consider $E = \mathbb{R}^d$ or $E = \mathbb{Z}^d$. We usually assume in this section that $E = \mathbb{R}^d$, with the understanding that all constructions can be easily extended to the discrete case. We assume that each configuration $\xi = (x_i), x_i \in E, i \in \mathbb{Z}^1$ (or $i \in \mathbb{Z}_+^1$ for $d > 1$), is locally finite. In other words, for every compact $K \subset E$, the number of particles in K , $\#_K(\xi) = \#\{x_i \in K\}$ is finite.

In order to introduce a σ -algebra of measurable subsets of X , we first define the cylinder sets. Let $B \subset E$ be a bounded Borel set and let $n \geq 0$. We call $C_n^B = \{\xi \in X : \#_B(\xi) = n\}$ a cylinder set. We define \mathcal{B} as a σ -algebra generated by all cylinder sets (i.e., \mathcal{B} is the minimal σ -algebra that contains all C_n^B).

Definition 1 A random point field is a triplet $(X, \mathcal{B}, \text{Pr})$, where Pr is a probability measure on (X, \mathcal{B}) .

It was observed in the 1960–1970s (see, e.g., Lenard (1973, 1975)), that in many cases the most convenient way to define a probability measure on (X, \mathcal{B}) is via the point correlation functions. Let $E = \mathbb{R}^d$, equipped with the underlying Lebesgue measure.

Definition 2 Locally integrable function $\rho_k : E^k \rightarrow \mathbb{R}_+^1$ is called a k -point correlation function of the random point field $(X, \mathcal{B}, \text{Pr})$ if, for any disjoint bounded Borel subsets A_1, \dots, A_m of E and for any $k_i \in \mathbb{Z}_+^1, i = 1, \dots, m, \sum_{i=1}^m k_i = k$, the following formula holds:

$$\begin{aligned} \mathbb{E} \prod_{i=1}^m \frac{(\#_{A_i})!}{(\#_{A_i} - k_i)!} \\ = \int_{A_1^{k_1} \times \dots \times A_m^{k_m}} \rho_k(x_1, \dots, x_k) dx_1 \cdots dx_k \quad [1] \end{aligned}$$

where by \mathbb{E} we denote the mathematical expectation with respect to Pr . In particular, $\rho_1(x)$ is the particle density, since

$$\mathbb{E} \#_A = \int_A \rho_1(x) dx$$

for any bounded Borel $A \subset E$. In general, $\rho_k(x_1, \dots, x_k)$ has the following probabilistic interpretation. Let $[x_i, x_i + dx_i], i = 1, \dots, k$, be infinitesimally small boxes around x_i , then $\rho_k(x_1, x_2, \dots, x_k) dx_1 \cdots dx_k$ is the probability to find a particle in each of these boxes.

In the discrete case $E = \mathbb{Z}^d$, the construction of a random point field is very similar. The probability space X and the σ -algebra \mathcal{B} are constructed essentially in the same way as before. Moreover, in the discrete case, the set of the countable configurations of particles can be identified with the set of all subsets of E . Therefore, $X = \{0, 1\}^E$, and \mathcal{B} is generated by the events $\{C_x, x \in E\}$, where $C_x = \{x \in \xi\}$. The k -point correlation function $\rho(x_1, \dots, x_k)$ is then just a probability that a configuration ξ contains the sites x_1, \dots, x_k . In other words, $\rho_k(x_1, \dots, x_k) = \Pr(\bigcap_{i=1}^k C_{x_i})$. In particular, the one-point correlation function $\rho_1(x), x \in \mathbb{Z}^d$, is the probability that a configuration contains the site x , that is, $\rho_1(x) = \Pr(C_x)$.

The problem of the existence and the uniqueness of a random point field defined by its correlation functions was studied by Lenard (1973–1975). It is not surprising that Lenard's papers revealed many parallels to the classical moment problem. In particular, the random point field is uniquely defined by its correlation functions if the distribution of random variables $\{\#_A\}$ for bounded Borel sets A is uniquely determined by its moments.

In this article we study a special class of random point fields introduced by Macchi (1975). To shorten the exposition, we give the definitions only in the continuous case $E = \mathbb{R}^d$. In the discrete case, the definitions are essentially the same.

Let $K: L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)$ be an integral locally trace-class operator. The last condition means that for any compact $B \subset \mathbb{R}^d$ the operator $K\chi_B$ is trace class, where $\chi_B(x)$ is an indicator of B . The kernel of K is defined up to a set of measure zero in $\mathbb{R}^d \times \mathbb{R}^d$. For our purposes, it is convenient to choose it in such a way that for any bounded measurable B and any positive integer n

$$\text{tr}((\chi_B K \chi_B)) = \int_B K(x, x) dx \quad [2]$$

We refer the reader to Soshnikov (2000, p. 927) for the discussion. We are now ready to define a determinantal (fermion) random point field on \mathbb{R}^d .

Definition 3 A random point field on E is said to be determinantal (or fermion) if its n -point correlation functions are of the form

$$\rho_n(x_1, \dots, x_n) = \det(K(x_i, x_j))_{1 \leq i \leq n} \quad [3]$$

Remark 1 If the kernel is Hermitian-symmetric, then the non-negativity of n -point correlation functions implies that the kernel $K(x, y)$ is non-negative definite and, therefore K must be a

non-negative operator. It should be noted, however, that there exist determinantal random point fields corresponding to non-Hermitian kernels (see, e.g., [18] later). The kernel $K(x, y)$ is usually called a correlation kernel of the determinantal random point process.

In the Hermitian case, the necessary and sufficient conditions on the operator K to define a determinantal random point field were established by Soshnikov (2000); see also Macchi (1975).

Theorem 1 *Hermitian locally trace class operator K on $L^2(E)$ determines a determinantal random point field if and only if $0 \leq K \leq 1$ (in other words, both K and $1 - K$ are non-negative operators). If the corresponding random point field exists, it is unique.*

The main technical part of the proof is the following proposition.

Proposition 1 *Let (X, \mathcal{B}, P) be a determinantal random point field with the Hermitian-symmetric correlation kernel K . Let f be a non-negative continuous function with compact support. Then*

$$\mathbb{E}e^{\langle \xi, f \rangle} = \det(\text{Id} - (1 - e^{-f})^{1/2} K (1 - e^{-f})^{1/2}) \quad [4]$$

where $\langle \xi, f \rangle$ is the value of the linear statistics defined by the test function f on the configuration $\xi = (x_i)$; in other words, $\langle \xi, f \rangle = \sum_i f(x_i)$.

Remark 2 The right-hand side (RHS) of [4] is well defined as the Fredholm determinant of a trace-class operator. Letting $f = \sum_{i=1}^k s_i \chi_{I_i}$, one obtains $\mathbb{E}e^{\langle \xi, f \rangle} = \mathbb{E} \prod_{i=1}^k z_i^{\#_{I_i}}$, with $z_i = e^{s_i}$. In this case, the left-hand side (LHS) of [4] becomes the generating function of the joint distribution of the counting random variables $\#_{I_i}, i = 1, \dots, k$.

Unfortunately, there are very few known results in the non-Hermitian case. In particular, the necessary and sufficient condition on K for the existence of the determinantal random point field with the non-Hermitian correlation kernel is not known.

We end this section with the introduction of the Janossy densities (a.k.a. density distributions, exclusion probability densities, etc.) of a random point field.

The term Janossy densities in the theory of random point processes was introduced by Srinivasan in 1969, who referred to the 1950 paper by Janossy on particle showers. Let us assume that all point correlation functions exist and are locally integrable, and let I be a bounded Borel subset of

\mathbb{R}^d . Intuitively, one can think of the Janossy density $\mathcal{J}_{k,I}(x_1, \dots, x_k)$, $x_1, \dots, x_k \in I$, as

$$\begin{aligned} \mathcal{J}_{k,I}(x_1, \dots, x_k) & \prod_{i=1}^k dx_i \\ &= \Pr\{\text{there are exactly } k \text{ particles in } I \text{ and} \\ & \quad \text{there is a particle in each of} \\ & \quad \text{the } k \text{ infinitesimal boxes } (x_i, x_i + dx_i), \\ & \quad i = 1, \dots, k\} \end{aligned} \quad [5]$$

To give a formal definition, we express point correlation functions in terms of Janossy densities and vice versa:

$$\begin{aligned} \rho_k(x_1, \dots, x_k) &= \sum_{j=1}^{\infty} \frac{1}{j!} \int_I \mathcal{J}_{k+j,I}(x_1, \dots, x_k, x_{k+1}, \dots, x_{k+j}) \\ & \quad \times dx_{k+1} \dots dx_{k+j} \end{aligned} \quad [6]$$

$$\begin{aligned} \mathcal{J}_{k,I}(x_1, \dots, x_k) &= \sum_{j=0}^{\infty} \frac{(-1)^j}{j!} \int_I \rho_{k+j}(x_1, \dots, x_k, x_{k+1}, \dots, x_{k+j}) \\ & \quad \times dx_{k+1} \dots dx_{k+j} \end{aligned} \quad [7]$$

A very useful property of the Janossy densities is that

$$\begin{aligned} \Pr\{\text{there are exactly } k \text{ particles in } I\} &= \frac{1}{k!} \int_I \mathcal{J}_{k,I}(x_1, \dots, x_k) dx_1 \dots dx_k \end{aligned} \quad [8]$$

In the case of determinantal random point fields, Janossy densities also have a determinantal form, namely

$$\begin{aligned} \mathcal{J}_{k,I}(x_1, \dots, x_k) &= \det(\text{Id} - K_I) \cdot \det(L_I(x_i, x_j))_{1 \leq i, j \leq k} \end{aligned} \quad [9]$$

In the last equation, K_I is the restriction of the operator K to the $L^2(I)$. In other words, $K_I(x, y) = \chi_I(x)K(x, y)\chi_I(y)$, where χ_I is the indicator of I . The operator L_I is expressed in terms of K_I as $L_I = (\text{Id} - K_I)^{-1}K_I$. For further results on the Janossy densities of determinantal random point processes we refer the reader to Soshnikov (2004) and references therein.

Examples of Determinantal Random Point Fields

Fermion Gas

Let $H = -d^2/dx^2 + V(x)$ be a Schrödinger operator with discrete spectrum on $L^2(E)$. We denote by

$\{\varphi_\ell\}_{\ell=0}^{\infty}$ an orthonormal basis of the eigenfunctions, $H\varphi_\ell = \lambda_\ell \cdot \varphi_\ell$, $\lambda_0 < \lambda_1 \leq \lambda_2 \leq \dots$. To define a Fermi gas, we consider the n th exterior power of H , $\wedge^n(H): \wedge^n(L^2(E)) \rightarrow \wedge^n(L^2(E))$, where $\wedge^n(L^2(E))$ is the space of square-integrable antisymmetric functions of n variables and $\wedge^n(H) = \sum_{i=1}^n (-d^2/dx_i^2 + V(x_i))$. The eigenstates of the Fermi gas are given by the normalized Slater determinants

$$\begin{aligned} \psi_{k_1, \dots, k_n}(x_1, \dots, x_n) &= \frac{1}{\sqrt{n!}} \sum_{\sigma \in S_n} (-1)^\sigma \prod_{i=1}^n \varphi_{k_i}(x_{\sigma(i)}) \\ &= \frac{1}{\sqrt{n!}} \det(\varphi_{k_i}(x_j))_{1 \leq i, j \leq n} \end{aligned} \quad [10]$$

where $0 \leq k_1 < k_2 < \dots < k_n$. A probability distribution of n particles in the Fermi gas is given by the squared absolute value of the eigenstate:

$$\begin{aligned} p(x_1, \dots, x_n) &= |\psi(x_1, \dots, x_n)|^2 \\ &= \frac{1}{n!} \det(\varphi_{k_i}(x_j))_{1 \leq i, j \leq n} \\ & \quad \times \det(\overline{\varphi_{k_j}(x_i)})_{1 \leq i, j \leq n} \\ &= \frac{1}{n!} \det(K_n(x_i, x_j))_{1 \leq i, j \leq n} \end{aligned} \quad [11]$$

where $K_n(x, y) = \sum_{i=1}^n \varphi_{k_i}(x)\overline{\varphi_{k_i}(y)}$ is the kernel of the orthogonal projector onto the subspace spanned by the n eigenfunctions $\{\varphi_{k_i}\}$ of H . The n -dimensional probability distribution [11] defines a determinantal random point field with n particles. The k -point correlation functions are given by

$$\begin{aligned} \rho_k^{(n)}(x_1, \dots, x_n) &= \frac{n!}{(n-k)!} \int p_n(x_1, \dots, x_n) \\ & \quad \times dx_{k+1} \dots dx_n \\ &= \det(K_n(x_i, x_j))_{1 \leq i, j \leq k} \end{aligned} \quad [12]$$

Random Matrix Models

Some of the most important ensembles of random matrices fall into the class of determinantal random point processes.

The archetypal ensemble of Hermitian random matrices is a so-called Gaussian unitary ensemble (GUE). Let us consider the space of $n \times n$ Hermitian matrices $\{A = (A_{ij})_{1 \leq i, j \leq n}, \text{Re}(A_{ij}) = \text{Re}(A_{ji}), \text{Im}(A_{ij}) = -\text{Im}(A_{ji})\}$. A GUE random matrix is defined by its probability distribution

$$P(dA) = \text{const}_n \cdot \exp(-\text{tr} A^2) dA \quad [13]$$

where dA is a Lebesgue measure, that is, $dA = \prod_{i < j} d\text{Re}(A_{ij}) d\text{Im}(A_{ij}) \prod_{k=1}^n dA_{kk}$. The eigenvalues of a random Hermitian matrix are real random

variables, whose joint probability distribution is a determinantal random point process of n particles on the real line. The correlation kernel has the Christoffel–Darboux form built from the Hermite polynomials.

The GUE ensemble of random matrices is invariant under the unitary transformation $A \rightarrow UAU^{-1}$, $U \in U(n)$. An important generalization of [13] that preserves the unitary invariance is

$$P(dA) = \text{const}_n \exp(-\text{tr} V(A)) dA \quad [14]$$

where, for example, $V(x)$ is a polynomial of even degree with positive leading coefficients. The correlation functions of the eigenvalues in [14] are again determinantal, and the Hermite polynomials in the correlation kernel have to be replaced by the orthonormal polynomials with respect to the weight $\exp(-V(x))$. For details, we refer the reader to the monographs by Mehta (2004) and Deift (2000).

There are many other ensembles of random matrices for which the joint distribution of the eigenvalues has determinantal point correlation functions: classical compact groups with respect to the Haar measure, complex non-Hermitian Gaussian random matrices, positive Hermitian random matrices of the Wishart type, and chains of correlated Hermitian matrices. We refer the reader to Soshnikov (2000) for more information.

Discrete Translation-Invariant Determinantal Random Point Fields

Let $g: \mathbb{T}^d \rightarrow [0, 1]$ be a Lebesgue-measurable function on the d -dimensional torus \mathbb{T}^d . Assume that $0 \leq g \leq 1$. A configuration ξ in \mathbb{Z}^d can be thought of as a 0–1 function on \mathbb{Z}^d , that is, $\xi(x) = 1$ if $x \in \xi$ and $\xi(x) = 0$ otherwise. We define a \mathbb{Z}^d -invariant probability measure Pr on the Borel sets of $X = \{0, 1\}^{\mathbb{Z}^d}$ in such a way that

$$\begin{aligned} \rho_k(x_1, \dots, x_k) &= \text{Pr}(\xi(x_1) = 1, \dots, \xi(x_k) = 1) \\ &:= \det(\hat{g}(x_i - x_j))_{1 \leq i, j \leq k} \end{aligned} \quad [15]$$

for $x_1, \dots, x_k \in \mathbb{Z}^d$. In the above formula, $\{g(n)\}$ are the Fourier coefficients of g , that is, $g(x) = \sum_n \hat{g}(n) e^{in \cdot x}$. It is clear from Definition 3 that [15] defines a determinantal random point field on \mathbb{Z}^d with the translation-invariant kernel $K(x, y) = \hat{g}(x - y)$. Below we discuss several examples that fall into this category. For further discussion we refer the reader to Lyons (2003) and Soshnikov (2000).

1. In the trivial case when g is identically a constant $p \in [0, 1]$, we obtain the i.i.d. Bernoulli probability measure.

2. The edges of the uniform spanning tree in \mathbb{Z}^2 parallel to the horizontal axis can be viewed as the determinantal random point field in \mathbb{Z}^2 with

$$g(x, y) = \frac{\sin^2 \pi x}{\sin^2 \pi x + \sin^2 \pi y}$$

Similarly, the edges of the uniform spanning forest in \mathbb{Z}^d parallel to the x_1 -axis correspond to the function

$$g(x_1, \dots, x_d) = \frac{\sin^2 \pi x_1}{\sum_{i=1}^d \sin^2 \pi x_i}$$

(the uniform spanning forest on \mathbb{Z}^d is a tree only for $d \leq 4$). The result is due to Burton and Pemantle (1993).

3. Let $d = 1$ and γ be a parameter between 0 and 1. Consider

$$g(x) = \frac{(1 - \gamma)^2}{|e^{2\pi i x} - \gamma|^2}$$

The corresponding probability measure is a renewal process and

$$K(n) = \hat{g}(n) = \frac{1 - \gamma}{1 + \gamma} \gamma^{|n|}$$

(see Soshnikov (2000)).

4. The process with $g(x) = \chi_I(x)$, where I is an arbitrary arc of a unit circle, appeared in the work of Borodin and Olshanski (2000). The corresponding correlation kernel is known as the discrete sine kernel. The determinantal random point process on \mathbb{Z}^1 with the discrete sine kernel describes the typical form of large Young diagrams “in the bulk” (see the next subsection).
5. The discrete sine correlation kernel with $g = \chi_{[0, 1/2]}$ appeared in the zig-zag process (Johansson 2002) derived from the uniform domino tilings in the plane. It corresponds to $g = \chi_{[0, 1/2]}$.

Determinantal Measures on Partitions

By a partition of $n = 1, 2, \dots$ we understand a collection of non-negative integers $\lambda = (\lambda_1, \dots, \lambda_m)$ such that $\lambda_1 + \dots + \lambda_m = n$ and $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_m$. We shall use a notation $\text{Par}(n)$ for the set of all partitions of n .

The Plancherel measure M_n on the set $\text{Par}(n)$ is defined as

$$M_n(\lambda) = \frac{(\dim \lambda)^2}{n!} \quad [16]$$

where $\dim \lambda$ is the dimension of the corresponding irreducible representation of the symmetric group

S_n . Let $\text{Par} = \bigsqcup_{n=0}^{\infty} \text{Par}(n)$. Consider a probability measure M^θ on Par

$$M^\theta(\lambda) = e^{-\theta} \frac{\theta^n}{n!} M_n(\lambda) \quad \text{where} \\ \lambda \in \text{Par}(n), \quad n = 0, 1, 2, \dots, \quad 0 \leq \theta < \infty \quad [17]$$

M^θ is called the Poissonization of the measures M_n . The analysis of the asymptotic properties of M_n and M^θ has been important in connection to the famous Ulam problem and related questions in representation theory.

It was shown by Borodin and Okounkov (2000), and, independently, Johansson (2001) that M^θ is a determinantal random point field. The corresponding correlation kernel K (in the so-called modified Frobenius coordinates) is a so-called discrete Bessel kernel on \mathbb{Z}^1 ,

$$K(x, y) = \begin{cases} \frac{\sqrt{\theta} J_{|x|-1/2}(2\sqrt{\theta}) J_{|y|+1/2}(2\sqrt{\theta}) - J_{|x|+1/2}(2\sqrt{\theta}) J_{|y|-1/2}(2\sqrt{\theta})}{|x| - |y|} & \text{if } xy > 0 \\ \sqrt{\theta} \frac{J_{|x|-1/2}(2\sqrt{\theta}) J_{|y|-1/2}(2\sqrt{\theta}) - J_{|x|+1/2}(2\sqrt{\theta}) J_{|y|+1/2}(2\sqrt{\theta})}{x - y} & \text{if } xy < 0 \end{cases} \quad [18]$$

where $J_x(\cdot)$ is the Bessel function of order x . One can observe that the kernel $K(x, y)$ is not Hermitian, but the restriction of this kernel to the positive and negative semiaxis is Hermitian.

M^θ is a special case of an infinite parameter family of probability measures on Par , called the Schur measures, and defined as

$$M(\lambda) = \frac{1}{Z} s_\lambda(x) s_\lambda(y) \quad [19]$$

where s_λ are the Schur functions, $x = (x_1, x_2, \dots)$ and $y = (y_1, y_2, \dots)$ are parameters such that

$$Z = \sum_{\lambda \in \text{Par}} s_\lambda(x) s_\lambda(y) = \prod_{i,j} (1 - x_i y_j)^{-1} \quad [20]$$

is finite and $\{x_i\}_{i=1}^{\infty} = \overline{\{y_i\}_{i=1}^{\infty}}$. It was shown by Okounkov (2001), that the Schur measures belong to the class of the determinantal random point fields.

NonIntersecting Paths of a Markov Process

Let $p_{t,s}(x, y)$ be the transition probability of a Markov process $\xi(t)$ on \mathbb{R} with continuous trajectories and let $(\xi_1(t), \xi_2(t), \dots, \xi_n(t))$ be n independent copies of the process. A classical result of Karlin and McGregor (1959) states that if n particles start at the positions $x_1^{(0)} < x_2^{(0)} < \dots < x_n^{(0)}$, then the

probability density of their joint distribution at time $t_1 > 0$, given that their paths have not intersected for all $0 \leq t \leq t_1$, is equal to

$$\pi_{t_1}(x_1^{(1)}, \dots, x_n^{(1)}) = \frac{1}{Z} \det(p_{0,t_1}(x_i^{(0)}, x_j^{(1)}))_{i,j=1}^n$$

provided the process $(\xi_1(t), \xi_2(t), \dots, \xi_n(t))$ in \mathbb{R}^n has a strong Markovian property.

Let $0 < t_1 < t_2 < \dots < t_{M+1}$. The conditional probability density that the particles are in the positions $x_1^{(1)} < x_2^{(1)} < \dots < x_n^{(1)}$ at time t_1 , at the positions $x_1^{(2)} < x_2^{(2)} < \dots < x_n^{(2)}$ at time t_2, \dots , at the positions $x_1^{(M)} < x_2^{(M)} < \dots < x_n^{(M)}$ at time t_M , given that at time t_{M+1} they are at the positions $x_1^{(M+1)} < x_2^{(M+1)} < \dots < x_n^{(M+1)}$ and their paths have not intersected, is then equal to

$$\pi_{t_1, t_2, \dots, t_M}(x_1^{(1)}, \dots, x_n^{(M)}) = \frac{1}{Z_n, M} \prod_{l=0}^M \det(p_{t_l, t_{l+1}}(x_i^{(l)}, x_j^{(l+1)}))_{i,j=1}^n \quad [21]$$

where $t_0 = 0$.

It is not difficult to show that [21] can be viewed as a determinantal random point process (see, e.g., Johansson (2003)).

The formulas of a similar type also appeared in the papers by Johansson, Prähofer, Spohn, Ferrari, Forrester, Nagao, Katori, and Tanemura in the analysis of polynuclear growth models, random walks on a discrete circle, and related problems.

Ergodic Properties

As before, let $(X, \mathcal{B}, \text{Pr})$ be a random point field with a one-particle space E . Hence, X is a space of the locally finite configurations of particles in E , \mathcal{B} a Borel σ -algebra of measurable subsets of X , and Pr a probability measure on (X, \mathcal{B}) . Throughout this section, we assume $E = \mathbb{R}^d$ or \mathbb{Z}^d . We define an action $\{T^t\}_{t \in E}$ of the additive group E on X in the following natural way:

$$T^t : X \rightarrow X, \quad (T^t \xi)_i = (\xi)_i + t \quad [22]$$

We recall that a random point field (X, \mathcal{B}, P) is called translation invariant if, for any $A \in \mathcal{B}$, any $t \in E$, $\text{Pr}(T^{-t}A) = \text{Pr}(A)$. The translation invariance of the correlation kernel $K(x, y) = K(x - y, 0) =: K(x - y)$ implies the translation invariance of k -point correlation functions

$$\rho_k(x_1 + t, \dots, x_k + t) = \rho_k(x_1, \dots, x_k) \\ \text{a.e. } k = 1, 2, \dots, \quad t \in E \quad [23]$$

which, in turn, implies the translation invariance of the random point field. The ergodic properties

of such point fields were studied by several mathematicians (Soshnikov 2000, Shirai and Takahashi, 2003, Lyons and Steif 2003). The first general result in this direction was obtained by Soshnikov (2000).

Theorem 2 *Let (X, B, P) be a determinantal random point field with a translation-invariant correlation kernel. Then the dynamical system $(X, B, P, \{T^t\})$ is ergodic, has the mixing property of any multiplicity and its spectra is absolutely continuous.*

We refer the reader to the article on ergodic theory for the definitions of ergodicity, mixing property, absolute continuous spectrum of the dynamical system, etc.

In the discrete case [15], $E = \mathbb{Z}^d$, more is known. Lyons and Steif (2003) proved that the shift dynamical system is Bernoulli, that is, it is isomorphic (in the ergodic theory sense) to an i.i.d. process. Under the additional conditions $\text{Spec}(K) \subset (0, 1)$ and $\sum_n |n| |K(n)|^2 < \infty$, Shirai and Takahashi (2003a) proved the uniform mixing property.

Gibbsian Properties

Costin and Lebowitz (1995) were the first to question the Gibbsian nature of the determinantal random point fields; they studied the continuous determinantal random point process on \mathbb{R}^1 with a so-called sine correlation kernel

$$K(x, y) = \frac{\sin(\pi(x - y))}{\pi(x - y)}$$

The first rigorous result (in the discrete case) was established by Shirai and Takahashi (2003b).

Theorem 3 *Let E be a countable discrete space and K a symmetric bounded operator on $\ell^2(E)$. Assume that $\text{Spec}(K) \subset (0, 1)$. Then (X, B, P) is a Gibbs measure with the potential U given by $U(x|\xi) = -\log(J(x, x) - \langle J_\xi^{-1} j_\xi^x, j_\xi^x \rangle)$, where $x \in E, \xi \in X$, $\{x\} \cap \xi = \emptyset$. Here $J(x, y)$ stands for the kernel of the operator $J = (\text{Id} - K)^{-1}K$, and we set $J_\xi = (J(y, z))_{y, z \in \xi}$ and $j_\xi^x = (J(x, y))_{y \in \xi}$.*

We recall that the Gibbsian property of the probability measure P on (X, B) means that

$$E[F|B_{\Lambda^c}](\xi) = \frac{1}{Z_{\Lambda, \xi}} \sum_{\eta \subset \Lambda} e^{-U(\eta|\xi_{\Lambda^c})} F(\eta \cup \xi_{\Lambda^c})$$

where Λ is a finite subset of E , B_{Λ^c} is the σ -algebra generated by the B -measurable functions with the support outside of Λ , $E[F|B_{\Lambda^c}]$ is the conditional

mathematical expectation of the integrable function F on (X, B, P) with respect to the σ -algebra B_{Λ^c} . The potential U is uniquely defined by the values of $U(x, \xi)$, as follows from the following recursive relation:

$$\begin{aligned} U(\{x_1, \dots, x_n\}|\xi) &= U(x_n|\{x_1, \dots, x_{n-1}\} \cup \xi) \\ &\quad + U(x_{n-1}|\{x_1, \dots, x_{n-2}\} \cup \xi) \\ &\quad + \dots + U(x_1|\xi) \end{aligned}$$

For additional information about the Gibbsian property, see Introductory Articles: Equilibrium Statistical Mechanics. Much less is known in the continuous case. Some generalized form of Gibbsian-ness, under quite restrictive conditions, was recently established by Georgii and Yoo (2004).

Central Limit Theorem for Counting Function

In this section, we discuss the central-limit theorem type results for the linear statistics. The first important result in this direction was established by Costin and Lebowitz in 1995, who proved the central-limit theorem for the number of particles in the growing box, $\#_{[-L, L]}$, $L \rightarrow \infty$, in the case of the determinantal random point process on \mathbb{R}^1 with the sine correlation kernel

$$K(x, y) = \frac{\sin(\pi(x - y))}{\pi(x - y)}$$

Below we formulate the Costin–Lebowitz theorem in its general form due to Soshnikov (1999, 2000).

Theorem 4 *Let E be a one-particle space, $\{0 \leq K_t \leq 1\}$ a family of locally trace-class operators in $\ell^2(E)$, $\{(X, B, P_t)\}$ a family of the corresponding determinantal random point fields in E , and $\{I_t\}$ a family of measurable subsets in E such that*

$$\begin{aligned} \text{Var} \#_{I_t} \\ = \text{tr}(K_t \cdot \chi_{I_t} - (K_t \cdot \chi_{I_t})^2) \rightarrow \infty \quad \text{as } t \rightarrow \infty \end{aligned} \quad [24]$$

Then the distribution of the normalized number of particles in I_t (with respect to P_t) converges to the normal law, that is,

$$\frac{\#_{I_t} - \mathbb{E} \#_{I_t}}{\sqrt{\text{Var} \#_{I_t}}} \xrightarrow{w} N(0, 1)$$

An analogous result holds for the joint distribution of the counting functions $\{\#_{I_{t_1}}, \dots, \#_{I_{t_k}}\}$, where $I_{t_1}^1, \dots, I_{t_k}^k$ are disjoint measurable subsets in E .

The proof of the Costin-Lebowitz theorem uses the k -point cluster functions. In the determinantal case, the cluster functions have a simple form

$$r_k(x_1, \dots, x_k) = (-1)^l \frac{1}{l!} \sum_{\sigma \in S_k} K(x_{\sigma(1)}, x_{\sigma(2)}) K(x_{\sigma(2)}, x_{\sigma(3)}) \cdots \times K(x_{\sigma(k)}, x_{\sigma(1)}) \quad [25]$$

The importance of the cluster function stems from the fact that the integrals of the k -point cluster function over the k -cube with a side l can be expressed as a linear combination of the first k cumulants of the counting random variable $\#_l$. In other words,

$$\int_{I \times \dots \times I} r_k(x_1, \dots, x_k) dx_1 \cdots dx_k = \sum_{l=1}^k \beta_{kl} C_l(\#_l) \quad [26]$$

It follows from [25] that the integral at the LHS of [26] equals, up to a factor $(-1)^l(l-1)!$, to the trace of the k th power of the restriction of K to I . This allows one to estimate the cumulants of the counting random variable $\#_l$. For details, we refer the reader to Soshnikov (2000). The central-limit theorem for a general class of linear statistics, under some technical assumptions on the correlation kernel was proved in Soshnikov (2002). Finally, we refer the reader to Soshnikov (2000) for the functional central-limit theorem for the empirical distribution function of the nearest spacings.

Generalizations: Immanantal and Pfaffian Point Processes

In this section, we discuss two important generalizations of the determinantal point processes.

Immanantal Processes

Immanantal random point processes were introduced by P Diaconis and S N Evans in 2000. Let λ be a partition of n . Denote by χ^λ the character of the corresponding irreducible representation of the symmetric group S_n . Let $K(x, y)$, be a non-negative-definite, Hermitian kernel. An immanantal random point process is defined through the correlation functions

$$\rho_k(x_1, \dots, x_k) = \sum_{\sigma \in S_n} \chi^\lambda(\sigma) \prod_{i=1}^n K(x_i, x_{\sigma(i)}) \quad [27]$$

In other words, the correlation functions are given by the immanants of the matrix with the entries $K(x_i, x_j)$. We will denote the RHS of [27] by $K^\lambda[x_1, \dots, x_n]$.

In the special case $\lambda = (1^n)$ (i.e., λ consists of n parts, all of which equal to 1), one obtains that $\chi^\lambda(\sigma) = (-1)^\sigma$, and $K^\lambda[x_1, \dots, x_n] = \det(K(x_i, x_j))$. Therefore, in the case $\lambda = (1^n)$ the random point process with the correlation functions [27] is a determinantal random point process. When $\lambda = (n)$ (i.e., the permutation has only one part, namely n) we have $\chi^\lambda = 1$ identically, and $K^\lambda[x_1, \dots, x_n] = \text{per}(K(x_i, x_j))$, the permanent of the matrix $K(x_i, x_j)$. The corresponding random point process is known as the boson random point process.

Pfaffian Processes

Let

$$K(x, y) = \begin{pmatrix} K_{11}(x, y) & K_{12}(x, y) \\ K_{21}(x, y) & K_{22}(x, y) \end{pmatrix}$$

be an antisymmetric 2×2 matrix-valued kernel, that is, $K_{ij}(x, y) = -K_{ji}(y, x)$, $i, j = 1, 2$. The kernel defines an integral operator acting on $L^2(E) \oplus L^2(E)$, which we assume to be locally trace class. A random point process on E is called Pfaffian if its point correlation functions have a Pfaffian form

$$\rho_k(x_1, \dots, x_k) = \text{pf}(K(x_i, x_j))_{i,j=1,\dots,k}, \quad k \geq 1 \quad [28]$$

The RHS of [28] is the Pfaffian of the $2k \times 2k$ antisymmetric matrix (since each entry $K(x_i, x_j)$ is a 2×2 block). Determinantal random point processes is a special case of the Pfaffian processes, corresponding to the matrix kernel of the form

$$K(x, y) = \begin{pmatrix} 0 & \tilde{K}(x, y) \\ -\tilde{K}(y, x) & 0 \end{pmatrix}$$

where \tilde{K} is a scalar kernel. The most well known examples of the Pfaffian random point processes, that cannot be reduced to determinantal form are $\beta = 1$ and $\beta = 4$ polynomial ensembles of random matrices and their limits (in the bulk and at the edge of the spectrum), as the size of a matrix goes to infinity.

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See also: Dimer Problems; Ergodic Theory; Growth Processes in Random Matrix Theory; Integrable Systems in Random Matrix Theory; Percolation Theory; Quantum Ergodicity and Mixing of Eigenfunctions; Random Matrix Theory in Physics; Random Partitions; Statistical Mechanics and Combinatorial Problems; Symmetry Classes in Random Matrix Theory.

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Diagrammatic Techniques in Perturbation Theory

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Introduction

Consider the dynamical system on \mathbb{R}^d described by the equation

$$\dot{u} = \frac{du}{dt} = G(u) + \varepsilon F(u) \quad [1]$$

where $F, G: \mathcal{S} \subset \mathbb{R}^d \rightarrow \mathbb{R}^d$ are analytic functions and ε a real (small) parameter. Suppose also that for $\varepsilon = 0$ a solution $u_0: \mathbb{R} \rightarrow \mathcal{S}$ (for some initial condition $u_0(0) = \bar{u}$) is known.

We look for a solution of [1] which is a perturbation of u_0 , that is, for a solution u which can be written in the form $u = u_0 + U$, with $U = O(\varepsilon)$ and $U(0) = \bar{U} \equiv u(0) - \bar{u}$. Then we consider the variational equation

$$\dot{U} = M(t)U + \Phi(t), \quad M_{ij}(t) = \partial_{u_i} G_j(u_0(t)) \quad [2]$$

where $\Phi(t) = \tilde{\Phi}(u_0(t), U)$, with $\tilde{\Phi}(u_0, U) = G(u_0 + U) - G(u_0) - \partial_u G(u_0)U + \varepsilon F(u_0 + U)$. By defining the Wronskian matrix W as the solution of the matrix equation $\dot{W} = M(t)W$ such that $W(0) = 1$ (the columns of W are given by d independent

solutions of the linear equation $\dot{u} = M(t)u$), we can write

$$U(t) = W(t)\bar{U} + W(t) \int_0^t d\tau W^{-1}(\tau)\Phi(\tau) \quad [3]$$

If we expect the solution U to be of order ε , we can try to write it as a Taylor series in ε , that is,

$$U(t) = \sum_{k=1}^{\infty} \varepsilon^k U^{(k)} \quad [4]$$

and, by inserting [4] into [3] and equating the coefficients with the same Taylor order, we obtain

$$U^{(k)}(t) = W(t)\bar{U}^{(k)} + W(t) \int_0^t d\tau W^{-1}(\tau)\Phi^{(k)}(\tau) \quad [5]$$

where $\Phi^{(k)}(t)$ is defined as

$$\begin{aligned} \Phi^{(1)}(t) &= F(u_0(t)) \\ \Phi^{(k)}(t) &= \sum_{p=2}^{\infty} \frac{1}{p!} \frac{\partial^p G}{\partial u^p}(u_0(t)) \sum_{k_1+\dots+k_p=k} U^{(k_1)} \dots U^{(k_p)} \\ &\quad + \sum_{p=1}^{\infty} \frac{1}{p!} \frac{\partial^p F}{\partial u^p}(u_0(t)) \\ &\quad \times \sum_{k_1+\dots+k_p=k-1} U^{(k_1)} \dots U^{(k_p)} \quad k \geq 2 \end{aligned} \quad [6]$$

Hence $\Phi^{(k)}(t)$ depends only on coefficients of orders strictly less than k . In this way, we obtain an algorithm useful for constructing the solution recursively, so that the problem is solved, up to (substantial) convergence problems.

Historical Excursus

The study of a system like [1] by following the strategy outlined above can be hopeless if we do not make some further assumptions on the types of motions we are looking for.

We shall see later, in a concrete example, that the coefficients $U^{(k)}(t)$ can increase in time, in a k -dependent way, thus preventing the convergence of the series for large t . This is a general feature of this class of problems: if no care is taken in the choice of the initial datum, the algorithm can provide a reliable description of the dynamics only for a very short time.

However, if one looks for solutions having a special dependence on time, things can work better. This happens, for instance, if one looks for quasiperiodic solutions, that is, functions which depend on time through the variable $\psi = \omega t$, with $\omega \in \mathbb{R}^N$ a vector with rationally independent components, that is such that $\omega \cdot \nu \neq 0$ for all $\nu \in \mathbb{Z}^N \setminus \{0\}$ (the dot denotes the standard inner product, $\omega \cdot \nu = \omega_1 \nu_1 + \dots + \omega_N \nu_N$). A typical problem of interest is: what happens to a quasiperiodic solution $u_0(t)$ when a perturbation εF is added to the unperturbed vector field G , as in [1]? Situations of this type arise when considering perturbations of integrable systems: a classical example is provided by planetary motion in celestial mechanics.

Perturbation series such as [4] have been extensively studied by astronomers in order to obtain a more accurate description of the celestial motions compared to that following from Kepler's theory (in which all interactions between planets are neglected and the planets themselves are considered as points). In particular, we recall the works of Newcomb and Lindstedt (series such as [4] are now known as Lindstedt series). At the end of the nineteenth century, Poincaré showed that the series describing quasiperiodic motions are well defined up to any perturbation order k (at least if the perturbation is a trigonometric polynomial), provided that the components of ω are assumed to be rationally independent: this means that, under this condition, the coefficients $U^{(k)}(t)$ are defined for all $k \in \mathbb{N}$. However, Poincaré also showed that, in general, the series are divergent; this is due to the fact that, as seen later, in the perturbation series small divisors $\omega \cdot \nu$ appear, which, even if they do not vanish, can be arbitrarily close to zero.

The convergence of the series can be proved indeed (more generally for analytic perturbations, or even those that are differentially smooth enough) by assuming on ω a stronger nonresonance condition, such as the Diophantine condition

$$|\omega \cdot \nu| > \frac{C_0}{|\nu|^\tau} \quad \forall \nu \in \mathbb{Z}^N \setminus \{0\} \quad [7]$$

where $|\nu| = |\nu_1| + \dots + |\nu_N|$, and C_0 and τ are positive constants. We note that the set of vectors satisfying [7] for some positive constant C_0 have full measure in \mathbb{R}^N provided one takes $\tau > N - 1$.

Such a result is part of the Kolmogorov–Arnold–Moser (KAM) theorem, and it was first proved by Kolmogorov in 1954, following an approach quite different from the one described here. New proofs were given in 1962 by Arnol'd and by Moser, but only very recently, in 1988, Eliasson gave a proof in which a bound C^k is explicitly derived for the coefficients $U^{(k)}(t)$, again implying convergence for ε to be small enough.

Eliasson's work was not immediately known widely, and only after publication of papers by Gallavotti and by Chierchia and Falcolini, in which Eliasson's ideas were revisited, did his work become fully appreciated. The study of perturbation series [4] employs techniques very similar to those typical of a very different field of mathematical physics, the quantum field theory, even if such an analogy was stressed and used to full extent only in subsequent papers.

The techniques have so far been applied to a wide class of problems of dynamical systems: a list of original results is given at the end.

A Paradigmatic Example

Consider the case $\mathcal{S} = \mathcal{A} \times \mathbb{T}^N$, with \mathcal{A} an open subset of \mathbb{R}^N , and let $\mathcal{H}_0: \mathcal{A} \rightarrow \mathbb{R}$ and $f: \mathcal{A} \times \mathbb{T}^N \rightarrow \mathbb{R}$ be two analytic functions. Then consider the Hamiltonian system with Hamiltonian $\mathcal{H}(A, \alpha) = \mathcal{H}_0(A) + \varepsilon f(A, \alpha)$. The corresponding equations describe a dynamical system of the form [1], with $u = (A, \alpha)$, which can be written explicitly:

$$\begin{cases} \dot{A} = -\varepsilon \partial_\alpha f(A, \alpha) \\ \dot{\alpha} = \partial_A \mathcal{H}_0(A) + \varepsilon \partial_A f(A, \alpha) \end{cases} \quad [8]$$

Suppose, for simplicity, $\mathcal{H}_0(A) = A^2/2$ and $f(A, \alpha) = f(\alpha)$, where $A^2 = A \cdot A$. Then, we obtain for α the following closed equation:

$$\ddot{\alpha} = -\varepsilon \partial_\alpha f(\alpha) \quad [9]$$

while A can be obtained by direct integration once [9] has been solved. For $\varepsilon = 0$, [9] gives trivially $\alpha = \alpha_0(t) \equiv \alpha_0 + \omega t$, where $\omega = \partial_A \mathcal{H}_0(A_0) = A_0$ is

called the rotation (or frequency) vector. Hence, for $\varepsilon=0$ all solutions are quasiperiodic. We are interested in the preservation of quasiperiodic solutions when $\varepsilon \neq 0$.

For $\varepsilon \neq 0$, we can write, as in [3],

$$\alpha = \alpha_0(t) + a(t), \quad a(t) = \sum_{k=1}^{\infty} \varepsilon^k a^{(k)}(t) \quad [10]$$

where $a^{(k)}$ is determined as the solution of the equation

$$a^{(k)} = t\bar{A}^{(k)} + \bar{a}^{(k)}(t) - \int_0^t d\tau \int_0^\tau d\tau' [\partial_\alpha f(\alpha(\tau'))]^{(k-1)} \quad [11]$$

with $[\partial_\alpha f(\alpha(\tau'))]^{(k-1)}$ expressed as in [6].

The quasiperiodic solutions with rotation vector ω could be written as a Fourier series, by expanding

$$a^{(k)}(t) = \sum_{\nu \in \mathbb{Z}^N} e^{i\nu \cdot \omega t} a_\nu^{(k)} \quad [12]$$

with ω as before. If the series [10], with the Taylor coefficients as in [12], exists, it will describe a quasiperiodic solution analytic in ε , and in such a case we say that it is obtained by continuation of the unperturbed one with rotation vector ω , that is $\alpha_0(t)$.

Suppose that the integrand $[\partial_\alpha f(\alpha(\tau'))]^{(k-1)}$ in [11] has vanishing average. Then the integral over τ' in [11] produces a quasiperiodic function, which in general has a nonvanishing average, so that the integral over τ produces a quasiperiodic function plus a term linear in t . If we choose $\bar{A}^{(k)}$ in [11] so as to cancel out exactly the term linear in time, we end up with a quasiperiodic function. In Fourier space, an explicit calculation gives, for all $\nu \neq 0$,

$$a_\nu^{(1)} = \frac{1}{(\omega \cdot \nu)^2} i\nu f_\nu$$

$$a_\nu^{(k)} = \frac{1}{(\omega \cdot \nu)^2} \sum_{p=1}^{\infty} \sum_{\substack{k_1+\dots+k_p=k-1 \\ \nu_0+\nu_1+\dots+\nu_p=\nu}} \frac{(i\nu_0)^{p+1}}{p!} a_{\nu_1}^{(k_1)} \dots a_{\nu_p}^{(k_p)} \quad [13]$$

$$k \geq 2$$

which again is suitable for an iterative construction of the solution. The coefficients $a_0^{(k)}$ are left undetermined, and we can fix them (arbitrarily) as identically vanishing.

Of course, the property that the integrand in [11] has zero average is fundamental; otherwise, terms increasing as powers of t would appear (the so-called secular terms). Indeed, it is easy to

realize that, if this happened, to order k terms proportional to t^{2k} could be present, thus requiring, at best, $|\varepsilon| < |t|^{-2}$ for convergence up to time t . This would exclude *a fortiori* the possibility of quasiperiodic solutions.

The aforementioned property of zero average can be verified only if the rotation vector is nonresonant, that is, if its components are rationally independent or, more particularly, if the Diophantine condition [7] is satisfied. Such a result was first proved by Poincaré, and it holds irrespective of how the parameters $\bar{a}^{(k)}$ appearing in [11] are fixed. This reflects the fact that quasiperiodic motions take place on invariant surfaces (KAM tori), which can be parameterized in terms of the angle variables $\alpha(t)$, so that the values $\bar{a}^{(k)}$ contribute to the initial phases, and the latter can be arbitrarily fixed.

The recursive equations [13] can be suitably studied by introducing a diagrammatic representation, as explained below.

Graphs and Trees

A (connected) graph G is a collection of points, called vertices, and lines connecting all of them. We denote with $V(G)$ and $L(G)$ the set of vertices and the set of lines, respectively. A path between two vertices is a minimal subset of $L(G)$ connecting the two vertices. A graph is planar if it can be drawn in a plane without graph lines crossing.

A tree is a planar graph G containing no closed loops (cycles); in other words, it is a connected acyclic graph. One can consider a tree G with a single special vertex ν_0 : this introduces a natural partial ordering on the set of lines and vertices, and one can imagine that each line carries an arrow pointing toward the vertex ν_0 . We can add an extra oriented line ℓ_0 connecting the special vertex ν_0 to another point which will be called the root of the tree; the added line will be called the root line. In this way, we obtain a rooted tree θ defined by $V(\theta) = V(G)$ and $L(\theta) = L(G) \cup \ell_0$. A labeled tree is a rooted tree θ together with a label function defined on the sets $V(\theta)$ and $L(\theta)$.

Two rooted trees which can be transformed into each other by continuously deforming the lines in the plane in such a way that the latter do not cross each other (i.e., without destroying the graph structure) will be said to be equivalent. This notion of equivalence can also be extended to labeled trees, simply by considering equivalent two labeled trees if they can be transformed into each other in such a way that the labels also match.

Given two vertices $v, w \in V(\theta)$, we say that $w \prec v$ if v is on the path connecting w to the root line. One

can identify a line with the vertices it connects; given a line $\ell = (v, w)$, one says that ℓ enters v and exits w . For each vertex v , we define the branching number as the number p_v of lines entering v .

The number of unlabeled trees with k vertices can be bounded by the number of random walks with $2k$ steps, that is, by 4^k .

The labels are as follows: with each vertex v we associate a mode label $\nu_v \in \mathbb{Z}^N$, and with each line we associate a momentum $\nu_\ell \in \mathbb{Z}^N$, such that the momentum of the line leaving the vertex v is given by the sum of the mode labels of all vertices preceding v (with v being included): if $\ell = (v', v)$ then $\nu_\ell = \sum_{w \preceq v} \nu_w$. Note that for a fixed unlabeled tree the branching labels are uniquely determined, and, for a given assignment of the mode labels, the momenta of the lines are also uniquely determined.

Define

$$V_v = \frac{(i\nu_v)^{p_v+1}}{p_v!} f_{\nu_v}, \quad g_\ell = \frac{1}{(\omega \cdot \nu_\ell)^2} \quad [14]$$

where the tensor V_v is referred to as the node factor of v and the scalar g_ℓ as the propagator of the line ℓ . One has $|f_\nu| \leq F e^{-\kappa|\nu|}$, for suitable positive constants F and κ , by the analyticity assumption. Then one can check that the coefficients $a_\nu^{(k)}$, defined in [12], for $\nu \neq 0$, can be expressed in terms of trees as

$$a_\nu^{(k)} = \sum_{\theta \in \Theta_\nu^{(k)}} \text{Val}(\theta) \quad [15]$$

$$\text{Val}(\theta) = \left(\prod_{v \in V(\theta)} V_v \right) \left(\prod_{\ell \in L(\theta)} g_\ell \right)$$

where $\Theta_\nu^{(k)}$ denotes the set of all inequivalent trees with k vertices and with momentum ν associated with the root line, while the coefficients $a_0^{(k)}$ can be fixed $a_0^{(k)} = 0$ for all $k \geq 1$, by the arbitrariness of the initial phases previously remarked. The property that $[\partial_\alpha f(\alpha(\tau'))]^{(k-1)}$ in [11] has zero average for all $k \geq 1$ implies that for all lines $\ell \in L(\theta)$ one has $g_\ell = (\omega \cdot \nu_\ell)^{-2}$ only for $\nu_\ell \neq 0$, whereas $g_\ell = 1$ for $\nu_\ell = 0$, so that the numerical values $\text{Val}(\theta)$ are well defined for all trees θ . If $a_0^{(k)} = 0$ for all $k \geq 1$, then $\nu_\ell \neq 0$ for all $\ell \in L(\theta)$.

The proof of [15] can be performed by induction on k . Alternatively, we can start from the recursive definition [13], whereby the trees naturally arise in the following way.

Represent graphically the coefficient $a_\nu^{(k)}$ as in Figure 1; to keep track of the labels k and ν , we assign k to the black bullet and ν to the line. For $k=1$, the black bullet is meant as a grey vertex (like the ones appearing in Figure 3).

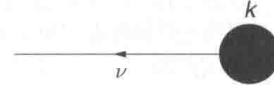


Figure 1 Graphical representation of $a_\nu^{(k)}$.

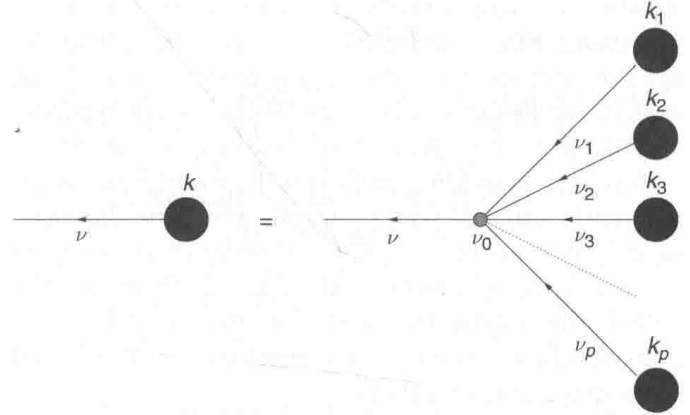


Figure 2 Graphical representation of the recursive equation [13].

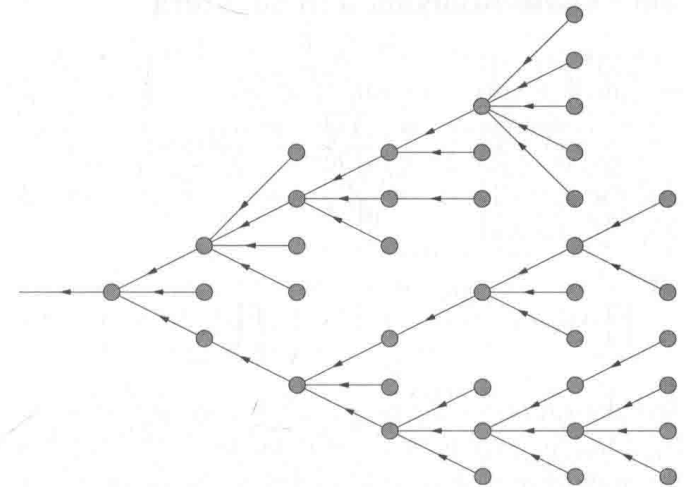


Figure 3 An example of tree to be summed over in [15] for $k=39$. The labels are not explicitly shown. The momentum of the root line is ν , so that the mode labels satisfy the constraint $\sum_{v \in V(\theta)} \nu_v = \nu$.

Then recursive equation [13] can be graphically represented as the diagram in Figure 2, provided that we associate with the (grey) vertex v_0 the node factor V_{v_0} , with $\nu_{v_0} = \nu_0$ and $p_{v_0} = p$ denoting the number of lines entering v_0 , and with the lines $\ell_i, i=1, \dots, p$, entering v_0 the momenta ν_{ℓ_i} , respectively. Of course, the sums over p and over the possible assignments of the labels $\{k_i\}_{i=1}^p$ and $\{\nu_i\}_{i=1}^p$ are understood. Each black bullet on the right-hand side of Figure 2, together with its exiting line looks like the diagram on the left-hand side, so that it represents $a_{\nu_i}^{(k_i)}, i=1, \dots, p$. Note that Figure 2 has to be interpreted in the following way: if one associates with the diagram as drawn in the right-hand side a numerical value (as

described above) and one sums all the values over the assignments of the labels, then the resulting quantity is precisely $a_\nu^{(k)}$.

The (fundamental) difference between the black bullets on the right- and left-hand sides is that the labels k_i of the latter are strictly less than k , hence we can iterate the diagrammatic decomposition simply by expressing again each $a_{\nu_i}^{(k_i)}$ as $a_{\nu_i}^{(k)}$ in [13], and so on, until one obtains a tree with k grey vertices and no black bullets; see Figure 3, where the labels are not explicitly written. This corresponds to the tree expansion [15].

Any tree appearing in [15] is an example of what physicists call a Feynman graph, while the diagrammatic rules one has to follow in order to associate to the tree θ its right numerical value $\text{Val}(\theta)$ are usually called the Feynman rules for the model under consideration. Such a terminology is borrowed from quantum field theory.

Multiscale Analysis and Clusters

Suppose we replace [9] with $\alpha = \varepsilon \partial_\alpha f(\alpha)$, so that no small divisors appear (that is, $g_\ell = 1$ in [14]). Then convergence is easily proved for ε small enough, since (by using the identity $\sum_{\nu \in V(\theta)} p_\nu = k - 1$ and the inequality $e^{-x} x^k / k! \leq 1$ for all $x \in \mathbb{R}_+$ and all $k \in \mathbb{N}$), one finds

$$\prod_{\nu \in V(\theta)} |V_\nu| \leq \left(\frac{4^2 F}{\kappa^2} \right)^k e^{-\kappa |\nu|/4} \left(\prod_{\nu \in V(\theta)} e^{-\kappa |\nu_\nu|/4} \right) \quad [16]$$

and the sum over the mode labels can be performed by using the exponential decay factors $e^{-\kappa |\nu_\nu|/4}$, while the sum over all possible unlabeled trees gives 4^k . In particular, analyticity in t follows.

Of course, the interesting case is when the propagators are present. In such a case, even if no division by zero occurs, as $\omega \cdot \nu_\ell \neq 0$ (by the assumed Diophantine condition [13] and the absence of secular terms discussed previously), the quantities $\omega \cdot \nu_\ell$ in [14] can be very small.

Then we can introduce a scale h characterizing the size of each propagator: we say that a line ℓ has scale $h_\ell = h \geq 0$ if $\omega \cdot \nu_\ell$ is of order $2^{-h} C_0$ and scale $h_\ell = -1$ if $\omega \cdot \nu_\ell$ is greater than C_0 (of course, a more formal definition can be easily envisaged, for which the reader is referred to the original papers). Then, we can bound $|\omega \cdot \nu_\ell| \geq 2^{-h} C_0$ for any $\ell \in L(\theta)$, and write

$$\begin{aligned} \prod_{\ell \in L(\theta)} |g_\ell| &\leq C_0^{-2k} \prod_{h=0}^{\infty} 2^{2h N_b(\theta)} \\ &\leq C_0^{-2k} 2^{2h_0 k} \exp \left(\sum_{h=h_0}^{\infty} 2 \log 2 h N_b(\theta) \right) \quad [17] \end{aligned}$$

where $N_b(\theta)$ is the number of lines in $L(\theta)$ with scale h and h_0 is a (so far arbitrary) positive integer. The problem is then reduced to that of finding an estimate for $N_b(\theta)$.

To identify which kinds of tree are the source of problems, we introduce the notion of a cluster and a self-energy graph. A cluster T with scale h_T is a connected set of nodes linked by a continuous path of lines with the same scale label h_T or a lower one and which is maximal, namely all the lines not belonging to T but connected to it have scales higher than h_T and at least one line in T has scale h_T . An inclusion relation is established between clusters, in such a way that the innermost clusters are the clusters with lowest scale, and so on. Each cluster T can have an arbitrary number of lines coming into it (entering lines), but only one or zero lines coming out from it (exiting line): lines of T which either enter or exit T are called external lines. A cluster T with only one entering line ℓ_T^2 and with one exiting line ℓ_T^1 such that one has $\nu_{\ell_T^1} = \nu_{\ell_T^2}$ will be called a self-energy graph (SEG) or resonance. In such a case, the line ℓ_T^1 is called a resonant line. Examples of clusters and SEGs are suggested by the bubbles in Figure 4; the mode labels are not represented, whereas the scales of the lines are explicitly written.

If $S_b(\theta)$ is the number of SEGs whose resonant lines have scales h , then $N_b^*(\theta) = N_b(\theta) - S_b(\theta)$ will denote the number of nonresonant lines with scale h .

A fundamental result, known as Siegel–Bryuno lemma, shows that, for some positive constant c , one has

$$N_b^*(\theta) \leq 2^{b/\tau c} \sum_{\nu \in V(\theta)} |\nu_\nu| \quad [18]$$

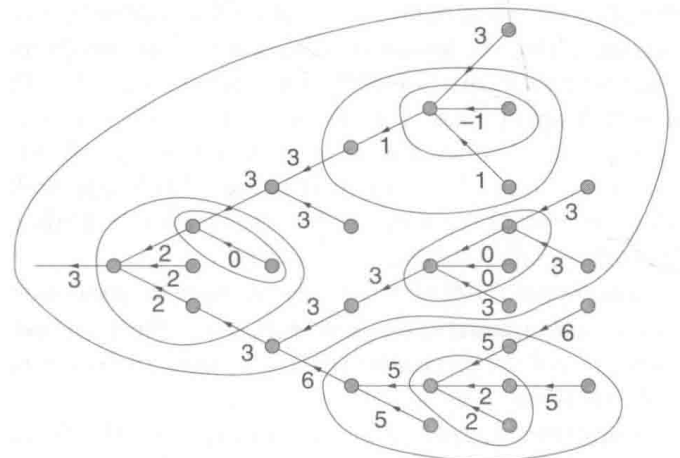


Figure 4 Examples of clusters and SEGs. Note that the tree itself is a cluster (with scale 6), and each of the two clusters with one entering and one exiting lines is a SEG only if the momenta of its external lines are equal to each other.

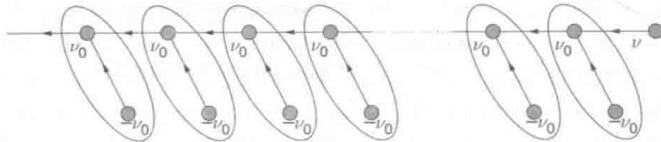


Figure 5 Example of tree whose value grows like a factorial.

which, if inserted into [17] instead of $N_b(\theta)$, would give a convergent series; then b_0 should be chosen in such a way that the sum of the series in [17] is less than, say, $\kappa \sum_{\nu \in V(\theta)} |\nu_\nu|/8$.

The bound [18] is a very deep one, and was originally proved by Siegel for a related problem (Siegel's problem), in which, in the formalism followed here, SEGs do not occur; such a bound essentially shows that accumulation of small divisors is possible only in the presence of SEGs. A possible tree with k vertices whose value can be proportional to some power of $k!$ is represented in Figure 5, where a chain of $(k-1)/2$ SEGs, k odd, is drawn with external lines carrying a momentum ν such that $\omega \cdot \nu \approx C_0 |\nu|^{-\tau}$.

In order to take into account the resonant lines, we have to add a factor $(\omega \cdot \nu_\ell)^{-2}$ for each resonant line ℓ . It is a remarkable fact that, even if there are trees whose value cannot be bounded as a constant to the power k , there are compensations (that is, partial cancellations) between the values of all trees with the same number of vertices, such that the sum of all such trees admits a bound of this kind.

The cancellations can be described graphically as follows. Consider a tree θ with a SEG T . Then take all trees which can be obtained by shifting the external lines of T , that is, by attaching such lines to all possible vertices internal to T , and sum together the values of all such trees. An example is given in Figure 6. The corresponding sum turns out to be proportional to $(\omega \cdot \nu)^2$, if ν is the momentum of the resonant line of T , and such a factor compensates exactly the propagator of this line. The argument above can be repeated for all SEGs: this requires a little care because there are SEGs which are inside some other SEGs. Again, for details and a more formal discussion, the reader is referred to original papers.

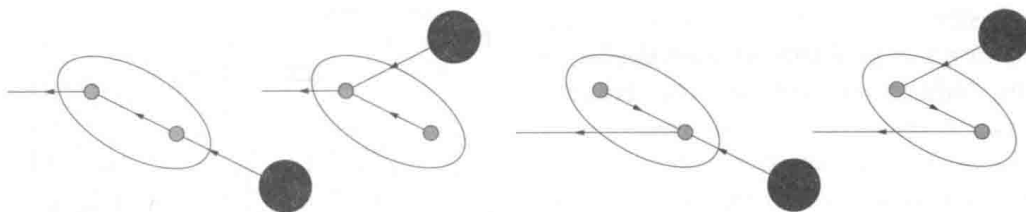


Figure 6 Example of SEGs whose values have to be summed together in order to produce the cancellation discussed in the text. The mode labels are all fixed.

The conclusion is that we can take into account the resonant lines: this simply adds an extra constant raised to the power k , so that an overall estimate C^k , for some $C > 0$, holds for $U^{(k)}(t)$, and the convergence of the series follows.

Other Examples and Applications

The discussion carried out so far proves a version of the KAM theorem, for the system described by [9], and it is inspired by the original papers by Eliasson (1996) and, mostly, by Gallavotti (1994).

Here we list some problems in which original results have been proved by means of the diagrammatic techniques described above, or by some variants of them. These are discussed in the following.

The first generalization one can think of is the problem of conservation in quasi-integrable systems of resonant tori (that is, invariant tori whose frequency vectors have rationally dependent components). Even if most of such tori disappear as an effect of the perturbation, some of them are conserved as lower-dimensional tori, which, generically, become of either elliptic or hyperbolic or mixed type according to the sign of ε and the perturbation. With techniques extending those described here (introducing also, in particular, a suitable resummation procedure for divergent series), this has been done by Gallavotti and Gentile; see Gallavotti *et al.* (2004) and Gallavotti and Gentile (2005) for an account.

An expansion like the one considered so far can be envisaged also for the motions occurring on the stable and unstable manifolds of hyperbolic lower-dimensional tori for perturbations of Hamiltonians describing a system of rotators (as in the previous case) plus n pendulum-like systems. In such a case, the function $G(u)$ has a less simple form. For $n=1$, one can look for solutions which depend on time through two variables, $\psi = \omega t$ and $x = e^{-gt}$, with $(\omega, g) \in \mathbb{R}^{N+1}$, and ω Diophantine as before and g related to the timescale of the pendulum. This has been worked out by Gallavotti (1994), and then used by Gallavotti *et al.* (1999) to study a class of three-timescale systems, in order to obtain a lower

bound on the homoclinic angles (i.e., the angles between the stable and unstable manifolds of hyperbolic tori which are preserved by the perturbation). The formalism becomes a little more involved, essentially because of the entries of the Wronskian matrix appearing in [5]. In such a case, the unperturbed solution $u_0(t)$ corresponds to the rotators moving linearly with rotation vector ω and the pendulum moving along its separatrix; a nontrivial fact is that if g_0 denotes the Lyapunov exponent of the pendulum in the absence of the perturbation, then one has to look for an expansion in $x = e^{-gt}$ with $g = g_0 + O(\varepsilon)$, because the perturbation changes the value of such an exponent.

The same techniques have also been applied to study the relation of the radius of convergence of the standard map, an area-preserving diffeomorphism from the cylinder to itself, which has been widely studied in the literature since the original papers by Greene and by Chirikov, both appeared in 1979, with the arithmetical properties of the rotation vector (which is, in this case, just a number). In particular, it has been proved that the radius of convergence is naturally interpolated through a function of the rotation number known as Bryuno function (which has been introduced by Yoccoz as the solution of a suitable functional equation completely independent of the dynamics); see Berretti and Gentile (2001) for a review of results of this and related problems.

Also the generalized Riccati equation $\dot{u} - iu^2 - 2if(\omega t) + i\varepsilon^2 = 0$, where $\omega \in \mathbb{T}^d$ is Diophantine and f is an analytic periodic function of $\psi = \omega t$, has been studied with the diagrammatic technique by Gentile (2003). Such an equation is related to two-level quantum systems (as first used by Barata), and existence of quasiperiodic solutions of the generalized Riccati equation for a large measure set \mathcal{E} of values of ε can be exploited to prove that the spectrum of the corresponding two-level system is pure point for those values of ε ; analogously, one can prove that, for fixed ε , one can impose some further nonresonance conditions on ω , still leaving a full measure set, in such a way that the spectrum is pure point. (We note, in addition, that, technically, such a problem is very similar to that of studying conservation of elliptic lower-dimensional tori with one normal frequency.)

Finally we mention a problem of partial differential equations, where, of course, the scheme

described above has to be suitably adapted: this is the study of periodic solutions for the nonlinear wave equation $u_{tt} - u_{xx} + mu = \varphi(u)$, with Dirichlet boundary conditions, where m is a real parameter (mass) and $\varphi(u)$ is a strictly nonlinear analytic odd function. Gentile and Mastropietro (2004) reproduced the result of Craig and Wayne for the existence of periodic solutions for a large measure set of periods, and, in a subsequent paper by the same authors with Procesi (2005), an analogous result was proved in the case $m=0$, which had previously remained an open problem in literature.

See also: Averaging Methods; Integrable Systems and Discrete Geometry; KAM Theory and Celestial Mechanics; Stability Theory and KAM.

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Dimer Problems

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Definitions

The dimer model arose in the mid-twentieth century as an example of an exactly solvable statistical mechanical model in two dimensions with a phase transition. It is used to model a number of physical processes: free fermions in 1 dimension, the two-dimensional Ising model, and various other two-dimensional statistical-mechanical models at restricted parameter values, such as the 6- and 8-vertex models and $O(n)$ models. A number of observable quantities such as the “height function” and densities of motifs have been shown to have conformal invariance properties in the scaling limit (when the lattice spacing tends to zero).

Recently, the model is also used as an elementary model of crystalline surfaces in \mathbb{R}^3 .

A dimer covering, or perfect matching, of a graph is a set of edges (“dimers”) which covers every vertex exactly once. In other words, it is a pairing of adjacent vertices (see Figure 1a which is a dimer covering of an 8×8 grid). Dimer coverings of a grid are sometimes represented as domino tilings, that is, tilings with 2×1 rectangles (Figure 1b). The dimer model is the study of the set of dimer coverings of a graph. Typically, the underlying graph is taken to be a regular lattice in two dimensions, for example, the square grid or the honeycomb lattice, or a finite part of such a lattice.

Dimer coverings of the honeycomb graph are in bijection with tilings of plane regions with 60° rhombi, also known as lozenges (see Figure 2). These tilings in turn are projections of piecewise-linear surfaces in \mathbb{R}^3 composed of unit squares in the 2-skeleton of \mathbb{Z}^3 . So one can think of honeycomb dimer coverings as modeling discrete surfaces in \mathbb{R}^3 . These surfaces are monotone in the sense that the orthogonal projection to the plane $P_{111} = \{(x, y, z) | x + y + z = 0\}$ is injective.

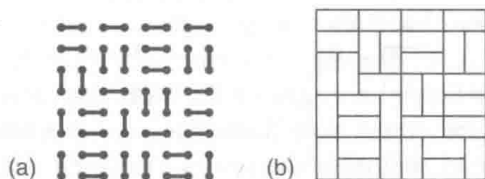


Figure 1 A dimer covering of a grid and the corresponding domino tiling.

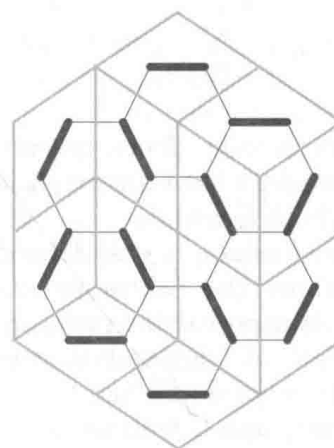


Figure 2 Honeycomb dimers (solid) and the corresponding “lozenge” tilings (gray).

Other models related to the dimer model are:

- The spanning tree model on planar graphs. The set of spanning trees on a planar graph is in bijection with the set of dimer coverings on an associated bipartite planar graph. Conversely, dimer coverings of a bipartite planar graph are in bijection with directed spanning trees on an associated graph.
- The Ising model on a planar graph with zero external field can be modeled with dimers on an associated planar graph.
- Plane partitions (three-dimensional versions of integer partitions). Viewing a plane partition along the $(1, 1, 1)$ -direction, one sees a lozenge tiling of the plane.
- Annihilating random walks in one dimension can be modeled with dimers on an associated planar graph.
- The monomer-dimer model, where one allows a certain density of holes (monomers) in a dimer covering. This model is unsolved at present, although some partial results have been obtained.

Gibbs Measures

The most general setting in which the dimer model can be solved is that of an arbitrary planar graph with energies on the edges. We define here the corresponding measure.

Let $G = (V, E)$ be a graph and $\mathcal{M}(G)$ the set of dimer coverings of G . Let \mathcal{E} be a real-valued function on the edges of G , with $\mathcal{E}(e)$ representing the energy associated to a dimer on the bond e . One defines the energy of a dimer covering as the sum of the energies of those bonds covered with dimers.

The partition function of the model on (G, \mathcal{E}) is then the sum

$$Z = \sum_{C \in \mathcal{M}(G)} e^{-\mathcal{E}(C)/kT}$$

where the sum is over dimer coverings. In what follows we will take $kT = 1$ for simplicity. Note that Z depends on both G and \mathcal{E} .

The partition function is well defined for a finite graph and defines the Gibbs measure, which is by definition the probability measure $\mu = \mu_{\mathcal{E}}$ on the set $\mathcal{M}(G)$ of dimer coverings satisfying $\mu(C) = (1/Z)e^{-\mathcal{E}(C)}$ for a covering C .

For an infinite graph G with fixed energy function \mathcal{E} , a Gibbs measure on $\mathcal{M}(G)$ is by definition any measure which is a limit of the Gibbs measures on a sequence of finite subgraphs which fill out G . There may be many Gibbs measures on an infinite graph, since this limit typically depends on the sequence of finite graphs. When G is an infinite periodic graph (and \mathcal{E} is periodic as well), it is natural to consider translation-invariant Gibbs measures; one can show that in the case of a bipartite, periodic planar graph the translation-invariant and ergodic Gibbs measures form a two-parameter family – see Theorem 3 below.

For a translation-invariant Gibbs measure ν which is a limit of Gibbs measures on an increasing sequence of finite graphs G_n , one can define the partition function per vertex of ν to be the limit

$$Z = \lim_{n \rightarrow \infty} Z(G_n)^{1/|G_n|}$$

where $|G_n|$ is the number of vertices of G_n . The free energy, or surface tension, of ν is $-\log Z$.

Combinatorics

Partition Function

One can compute the partition function for dimer coverings on a finite planar graph G as the Pfaffian (square root of the determinant) of a certain antisymmetric matrix, the Kasteleyn matrix. The Kasteleyn matrix is an oriented adjacency matrix of G , indexed by the vertices V : orient the edges of a graph embedded in the plane so that each face has an odd number of clockwise oriented edges. Then define $K = (K_{vv'})$ with

$$K_{vv'} = \pm e^{-\mathcal{E}(vv')}$$

if G has an edge vv' , with a sign according to the orientation of that edge, and $K_{vv'} = 0$ if v, v' are not

adjacent. We then have the following result of Kasteleyn:

Theorem 1 $Z = |\text{Pf}(K)| = \sqrt{|\det K|}$.

Here $\text{Pf}(K)$ denotes the Pfaffian of K .

Such an orientation of edges (which always exists for planar graphs) is called a Kasteleyn orientation; any two such orientations can be obtained from one another by a sequence of operations consisting of reversing the orientations of all edges at a vertex.

If G is a bipartite graph, that is, the vertices can be colored black and white with no neighbors having the same color, then the Pfaffian of K is the determinant of the submatrix whose rows index the white vertices and columns index the black vertices. For bipartite graphs, instead of orienting the edges one can alternatively multiply the edge weights by a complex number of modulus 1, with the condition that the alternating product around each face (the first, divided by the second, times the third, as so on) is real and negative.

For nonplanar graphs, one can compute the partition function as a sum of Pfaffians; for a graph embedded on a surface of Euler characteristic χ , this requires in general $2^{2-\chi}$ Pfaffians.

Local Statistics

The inverse of the Kasteleyn matrix can be used to compute the local statistics, that is, the probability that a given set of edges occurs in a random dimer covering (random with respect to the Gibbs measure μ).

Theorem 2 Let $S = \{(v_1, v_2), \dots, (v_{2k-1}, v_{2k})\}$ be a set of edges of G . The probability that all these edges occur in a μ -random covering is

$$\Pr(S) = \left(\prod_{i=1}^k K_{v_{2i-1}, v_{2i}} \right) \text{Pf}_{2k \times 2k}((K^{-1})_{v_i, v_j})$$

Again, for bipartite graphs the Pfaffian can be made into a determinant.

Heights

Bipartite graphs Suppose G is a bipartite planar graph. A 1-form on G is simply a function on the set of oriented edges which is antisymmetric with respect to reversing the edge orientation: $f(-e) = -f(e)$ for an edge e . A 1-form can be identified with a flow: just flow by $f(e)$ along oriented edge e . The divergence of the flow f is then d^*f . Let Ω be the space of flows on edges of G , with divergence 1 at each white vertex and divergence -1 at each black vertex, and such that the flow along each edge from white to black is in $[0, 1]$. From a dimer covering M one can construct such a flow $\omega(M) \in \Omega$: just flow

one unit along each dimer, and zero on the remaining edges. The set Ω is a convex polyhedron in \mathbb{R}^E and its vertices can be seen to be exactly the dimer coverings.

Given any two flows $\omega_1, \omega_2 \in \Omega$, their difference is a divergence-free flow. Its dual $(\omega_1 - \omega_2)^*$ (or conjugate flow) defined on the planar dual of G is therefore the gradient of a function h on the faces of G , that is, $(\omega_1 - \omega_2)^* = dh$, where h is well defined up to an additive constant.

When ω_1 and ω_2 come from dimer coverings, h is integer valued, and is called the height difference of the coverings. The level sets of the function h are just the cycles formed by the union of the two matchings. If we fix a “base point” covering ω_0 and a face f_0 of G , we can then define the height function of any dimer covering (with flow ω) to be the function h with value zero at f_0 and which satisfies $dh = (\omega - \omega_0)^*$.

Nonbipartite graphs On a nonbipartite planar graph the height function can be similarly defined modulo 2. Fix a base covering ω_0 ; for any other covering ω , the superposition of ω_0 and ω is a set of cycles and doubled edges of G ; the function h is constant on the complementary components of these cycles and changes by 1 mod 2 across each cycle. We can think of the height modulo 2 as taking two values, or spins, on the faces of G , and the dimer chains are the spin-domain boundaries. In particular, dimers on a nonbipartite graph model can in this way model the Ising model on an associated dual planar graph.

Thermodynamic Limit

By periodic planar graph we mean a graph G , with energy function on edges, for which translations by elements of \mathbb{Z}^2 or some other rank-2 lattice $\Gamma \subset \mathbb{R}^2$ are isomorphisms of G preserving the edge energies, and such that the quotient G/\mathbb{Z}^2 is a finite graph. Without loss of generality we can take $\Gamma = \mathbb{Z}^2$. The standard example is $G = \mathbb{Z}^2$ with $\mathcal{E} \equiv 0$, which we refer to as “dimers on the grid.” However, other examples display different global behaviors and so it is worthwhile to remain in this generality.

For a periodic planar graph G , an ergodic probability measure on $\mathcal{M}(G)$ is one which is translation invariant (the measure of a set is the same as any \mathbb{Z}^2 -translate of that set) and whose invariant subsets have measure 0 or 1.

We will be interested in probability measures which are both ergodic and Gibbs (we refer to them as ergodic Gibbs measures, dropping the term “probability”). When G is bipartite, there are multiple ergodic Gibbs measures (see Theorem 3

below). When G is nonbipartite, it is conjectured that there is a single ergodic Gibbs measure.

In the remainder of this section we assume that G is bipartite, and assume also that the \mathbb{Z}^2 -action preserves the coloring of the edges as black and white (simply pass to an index-2 sublattice if not).

For integer $n > 0$ let $G_n = G/n\mathbb{Z}^2$, a finite graph on a torus (in other words, with periodic boundary conditions). For a dimer covering M of G_n , we define $(h_x, h_y) \in \mathbb{Z}^2$ to be the horizontal and vertical height change of M around the torus, that is, the net flux of $\omega(M) - \omega_0$ across a horizontal, respectively vertical, cut around the torus (in other words, h_x, h_y are the horizontal and vertical periods around the torus of the 1-form $\omega(M) - \omega_0$). The characteristic polynomial $P(z, w)$ of G is by definition

$$P(z, w) = \sum_{M \in \mathcal{M}(G_1)} e^{-\mathcal{E}(M)} z^{h_x} w^{h_y} (-1)^{h_x h_y}$$

here the sum is over dimer coverings M of $G_1 = G/\mathbb{Z}^2$, and h_x, h_y depend on M . The polynomial P depends on the base point ω_0 only by a multiplicative factor involving a power of z and w . From this polynomial most of the large-scale behavior of the ergodic Gibbs measures can be extracted.

The Gibbs measure on G_n converges as $n \rightarrow \infty$ to the (unique) ergodic Gibbs measure μ with smallest free energy $F = -\log Z$. The unicity of this measure follows from the strict concavity of the free energy of ergodic Gibbs measures as a function of the slope, see below. The free energy F of the minimal free energy measure is

$$F = -\frac{1}{(2\pi i)^2} \int_{S^1 \times S^1} \log P(z, w) \frac{dz}{z} \frac{dw}{w}$$

that is, minus the Mahler measure of P .

For any translation-invariant measure ν on $\mathcal{M}(G)$, the average slope (s, t) of the height function for ν -almost every tiling is by definition the expected horizontal and vertical height change over one fundamental domain, that is, $s = \mathbb{E}[h(f + (1, 0)) - h(f)]$ and $t = \mathbb{E}[h(f + (0, 1)) - h(f)]$ where f is any face. This quantity (s, t) lies in the Newton polygon of $P(z, w)$ (the convex hull in \mathbb{R}^2 of the set of exponents of monomials of P). In fact, the points in the Newton polygon are in bijection with the ergodic Gibbs measures on $\mathcal{M}(G)$:

Theorem 3 *When G is a periodic bipartite planar graph, any ergodic Gibbs measure has average slope (s, t) lying in $N(P)$. Moreover, for every point $(s, t) \in N(P)$ there is a unique ergodic Gibbs measure $\mu(s, t)$ with that average slope.*

In particular, this gives a complete description of the set of all ergodic Gibbs measures. The ergodic Gibbs measure $\mu(s, t)$ of slope (s, t) can be obtained as the limit of the Gibbs measures on G_n , when one conditions the configurations to have a particular slope approximating (s, t) .

Ronkin Function and Surface Tension

The Ronkin function of P is a map $R: \mathbb{R}^2 \rightarrow \mathbb{R}$ defined for $(B_x, B_y) \in \mathbb{R}^2$ by

$$R(B_x, B_y) = \frac{1}{(2\pi i)^2} \int_{S^1 \times S^1} \log P(ze^{B_x}, we^{B_y}) \frac{dz}{z} \frac{dw}{w}$$

The Ronkin function is convex and its graph is piecewise linear on the complement of the amoeba $A(P)$ of P , which is the image of the zero set $\{(z, w) \in \mathbb{C}^2 \mid P(z, w) = 0\}$ under the map $(z, w) \mapsto (\log |z|, \log |w|)$ (see Figures 3 and 4 for an example).

The free energy $F(\mu(s, t))$ of $\mu(s, t)$, as a function of $(s, t) \in N(P)$, is the Legendre dual of the Ronkin function of $P(z, w)$: we have

$$F(\mu(s, t)) = R(B_x, B_y) - sB_x - tB_y$$

where

$$s = \frac{\partial R(B_x, B_y)}{\partial B_x}, \quad t = \frac{\partial R(B_x, B_y)}{\partial B_y}$$

The continuous map $\nabla R: \mathbb{R}^2 \rightarrow N(P)$ which takes (B_x, B_y) to (s, t) is injective on the interior of $A(P)$, collapses each bounded complementary component of $A(P)$ to an integer point in the interior of $N(P)$, and collapses each unbounded complementary component of $A(P)$ to an integer point on the boundary of $N(P)$.

Under the Legendre duality, the facets in the graph of the Ronkin function (i.e., maximal regions

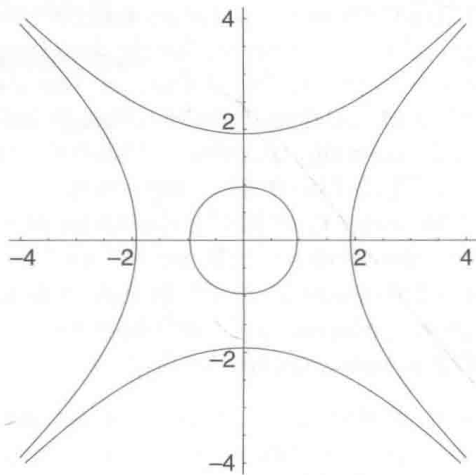


Figure 3 The amoeba of $P(z, w) = 5 + z + 1/z + w + 1/w$, which is the characteristic polynomial for dimers on the periodic “square-octagon” lattice.



Figure 4 Minus the Ronkin function of $P(z, w) = 5 + z + 1/z + w + 1/w$.

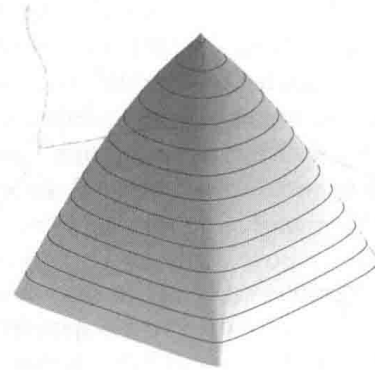


Figure 5 (Negative of) the free energy for dimers on the square-octagon lattice.

on which R is linear) give points of nondifferentiability of the free energy F , as defined on $N(P)$. We refer to these points of nondifferentiability as “cusps.” Cusps occur only at integer slopes (s, t) (see Figure 5 for the free energy associated to the Ronkin function in Figure 4).

By Theorem 3, the coordinates (B_x, B_y) can also be used to parametrize the set of Gibbs measures $\mu(s, t)$ (but only those with slope (s, t) in the interior of $N(P)$ or on the corners of $N(P)$ and boundary integer points). This parametrization is not one-to-one since when (B_x, B_y) varies in a complementary component of the amoeba, the measure $\mu(s, t)$ does not change. On the interior of the amoeba the parametrization is one-to-one.

The remaining Gibbs measures, whose slopes are on the boundary of $N(P)$, can be obtained by taking limits of (B_x, B_y) along the “tentacles” of the amoeba.

Phases

The Gibbs measures $\mu(s, t)$ can be partitioned into three classes, or phases, according to the behavior of the fluctuations of the height function. If we measure the height at two distant points x_1 and x_2 in G , the average height difference, $E[h(x_1) - h(x_2)]$, is a linear function of $x_1 - x_2$ determined by the average slope of the measure. The height fluctuation is defined to be the random variable $h(x_1) - h(x_2) - E[h(x_1) - h(x_2)]$. This random variable depends on

the two points and we are interested in its behavior when x_1 and x_2 are far apart.

We say $\mu(s, t)$ is

1. “Frozen” if the height fluctuations are bounded almost surely.
2. “Rough” (or “liquid”) if the covariance in the height function $\mathbb{E}[h(x_1)h(x_2)] - \mathbb{E}[h(x_1)]\mathbb{E}[h(x_2)]$ is unbounded as $|x_1 - x_2| \rightarrow \infty$.
3. “Smooth” (or “gaseous”) if the covariance of the height function is bounded but the height fluctuations are unbounded.

The height fluctuations can be related to the decay of the entries of K^{-1} , which are in turn related to the decay of the Fourier coefficients of $1/P$. In particular, we have

Theorem 4 *The measure $\mu(s, t)$ is respectively frozen, rough, or smooth according to whether $(B_x, B_y) = (\nabla R)^{-1}(s, t)$ is in the closure of an unbounded complementary component of $\mathbb{A}(p)$, in the interior of $\mathbb{A}(P)$, or in the closure of a bounded component of $\mathbb{A}(P)$.*

The characteristic polynomials P which occur in the dimer model are not arbitrary: their algebraic curves $\{P=0\}$ are all of a special type known as Harnack curves, which are characterized by the fact that the map from the zero-set of P in \mathbb{C}^2 to its amoeba in \mathbb{R}^2 is at most two-to-one. In fact:

Theorem 5 *By varying the edge energies all Harnack curves can be obtained as the characteristic polynomial of a planar dimer model.*

Local Statistics

In the thermodynamic limit (on a periodic planar graph), local statistics of dimer coverings for the Gibbs measure of minimal free energy can be obtained from the limit of the inverse of the Kasteleyn matrix on the finite toroidal graphs G_n . This in turn can be computed from the Fourier coefficients of $1/P$.

As an example, let G be the square grid \mathbb{Z}^2 and take $\mathcal{E}=0$ (which corresponds to the uniform measure on configurations for finite graphs). An appropriate choice of signs for the Kasteleyn matrix is to put weights 1, -1 on alternate horizontal edges and i , $-i$ on alternate vertical edges in such a way that around each white vertex the weights are cyclically 1, i , -1 , $-i$. For this choice of signs we have

$$K_{(0,0),(x,y)}^{-1} = \frac{1}{(2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} \frac{e^{-i(\theta x + \phi y)} d\theta d\phi}{2 \sin \theta + 2i \sin \phi}$$

This integral can be evaluated explicitly (see Figure 6 for values of $K_{(0,0),(x,y)}^{-1}$ near the origin; by

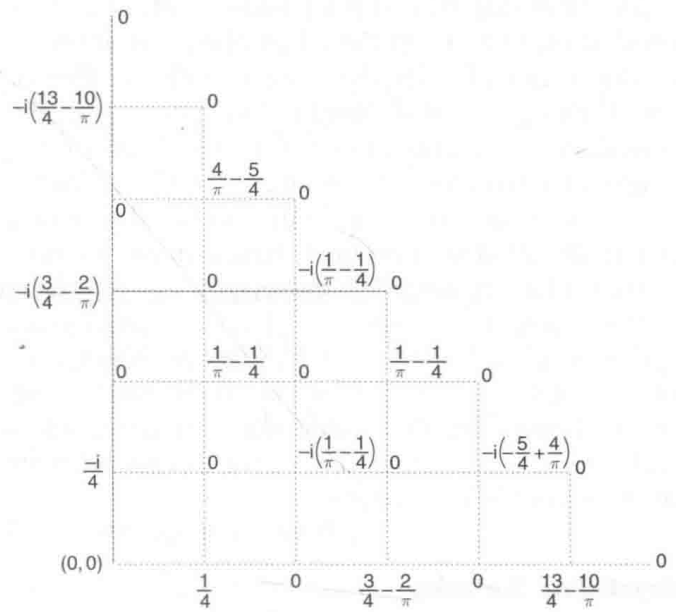


Figure 6 Values of K^{-1} on \mathbb{Z}^2 with zero energies.

translation invariance $K_{(x',y'),(x,y)}^{-1} = K_{(0,0),(x-x',y-y')}^{-1}$ and values in other quadrants can be obtained by $K_{(0,0),(x,y)}^{-1} = -iK_{(0,0),(-y,x)}^{-1}$.

As a sample computation, using Theorem 2, the probability that the dimer covering the origin points to the right and, simultaneously, the one covering $(0, 1)$ points upwards is

$$K_{(0,0),(1,0)} K_{(0,2),(0,1)} \det \begin{pmatrix} K_{(0,0),(1,0)}^{-1} & K_{(0,0),(0,1)}^{-1} \\ K_{(0,2),(1,0)}^{-1} & K_{(0,2),(0,1)}^{-1} \end{pmatrix} = 1 \cdot (-i) \cdot \det \begin{pmatrix} \frac{1}{4} & \frac{-i}{4} \\ -\frac{1}{4} + \frac{1}{\pi} & \frac{1}{4} \end{pmatrix} = \frac{1}{4\pi}$$

Another computation which follows is the decay of the edge covariances. If e_1, e_2 are two edges at distance d , then $\Pr(e_1 \& e_2) - \Pr(e_1)\Pr(e_2)$ decays quadratically in $1/d$, since $K^{-1}((0, 0), (x, y))$ decays like $1/(|x| + |y|)$.

Scaling Limits

The scaling limit of the dimer model is the limit when the lattice spacing tends to zero.

Let us define the scaling limit in the following way. Let $\epsilon\mathbb{Z}^2$ be the square grid scaled by ϵ , so the lattice mesh size is ϵ . Fix a Jordan domain $U \subset \mathbb{R}^2$ and consider for each ϵ a subgraph U_ϵ of $\epsilon\mathbb{Z}^2$, bounded by a simple polygon, which tends to U as $\epsilon \rightarrow 0$. We are interested in limiting properties of random dimer coverings of U_ϵ , in the limit as $\epsilon \rightarrow 0$, for example, the fluctuations of the height function and edge densities.

The limit depends on the (sequence of) boundary conditions, that is, on the exact choice of approximating regions U_ϵ . By changing U_ϵ one can change the limiting rescaled height function along the boundary. It is conjectured that the limit of the height function along the boundary of U_ϵ (scaled by $\epsilon \dots$ and assuming this limit exists) determines essentially all of the limiting behavior in the interior, in particular the limiting local statistics.

Therefore, let u be a real-valued continuous function on the boundary of U . Consider a sequence of subgraphs U_ϵ of $\epsilon\mathbb{Z}^2$, as $\epsilon \rightarrow 0$ as above, and whose height function along the boundary, when scaled by ϵ , is approximating u . We discuss the limit of the model in this setting.

Crystalline Surfaces

The height function allows us to view dimer coverings as random surfaces in \mathbb{R}^3 : to a dimer covering of G , one associates the graph of its height function, extended in a piecewise linear fashion over the edges and faces of the dual G^* . These surfaces are then piecewise linear random surfaces, which resemble crystal surfaces in the sense that microscopically (on the scale of the lattice) they are rough, whereas their long-range behavior is smooth and faceted, as we now describe.

In the scaling limit, boundary conditions as described in the last paragraph of the previous section are referred to as “wire-frame” boundary conditions, since the graph of the height function can be thought of as a (random) surface spanning the wire frame defined by its boundary values.

In the scaling limit, there is a law of large numbers which says that the Gibbs measure on random surfaces (which is unique since we are dealing with a finite graph) concentrates, for fixed wire-frame boundary conditions, on a single surface S_0 . That is, as the lattice spacing ϵ tends to zero, with probability tending to 1 the random surface lies close to a limiting surface S_0 . The surface S_0 is the unique surface which minimizes the total surface tension, or free energy, for its fixed boundary values, that is, minimizes the integral over the surface of the $F(\mu(s, t))$, where (s, t) is the slope of the surface at the point being integrated over. Existence and unicity of the minimizer follow from the strict convexity of the free energy/surface tension as a function of the slope.

At a point where the free energy has a cusp, the crystal surface S_0 will in general have a facet, that is, a region on which it is linear. Outside of the facets, one expects that S_0 is analytic, since the free energy is analytic outside the cusps.

Fluctuations

While the scaled height function ϵh in the scaling limit converges to its mean value h_0 (whose graph is the surface S_0), the fluctuations of the unrescaled height function $h - (1/\epsilon)h_0$ will converge in law to a random process on U .

In the simplest setting, that of honeycomb dimers with $\mathcal{E} \equiv 0$, and in the absence of facets, the height fluctuations converge to a continuous Gaussian process, the image of the Gaussian free field on the unit disk \mathbb{D} under a certain diffeomorphism Φ (depending on h_0) of \mathbb{D} to U .

In the particular case $h_0 = 0$, Φ is the Riemann map from \mathbb{D} to U and the law of the height fluctuations is just the Gaussian free field on U (defined to be the Gaussian process whose covariance kernel is the Dirichlet Green's function). The conformal invariance of the Gaussian free field is the basis for a number of conformal invariance properties of the honeycomb dimer model.

Densities of Motifs

Another observable of interest is the density field of a motif. A motif is a finite collection of edges, taken up to translation. For example, consider, for the square grid, the “L” motif consisting of a horizontal domino and a vertical domino aligned to form an “L,” which we showed above to have a density $1/4\pi$ in the thermodynamic limit. The probability of seeing this motif at any given place is $1/4\pi$. However, in the scaling limit one can ask about the fluctuations of the occurrences of this motif: in a large ball around a point x , what is the distribution of $N_L - A/4\pi$, where N_L is the number of occurrences of the motif, and A is the area of the ball? These fluctuations form a random field, since there is a long-range correlation between occurrences of the motif.

It is known that on \mathbb{Z}^2 , for the minimal free energy ergodic Gibbs measure, the rescaled density field

$$\frac{1}{\sqrt{A}} \left(N_L - \frac{A}{4\pi} \right)$$

converges as $\epsilon \rightarrow 0$ weakly to a Gaussian random field which is a linear combination of a directional derivative of the Gaussian free field and an independent white noise. A similar result holds for other motifs.

The joint distribution of densities of several motifs can also be shown to be Gaussian.

See also: Combinatorics: Overview; Determinantal Random Fields; Growth Processes in Random Matrix Theory; Statistical Mechanics and Combinatorial Problems; Statistical Mechanics of Interfaces.

Further Reading

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Dirac Fields in Gravitation and Nonabelian Gauge Theory

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Introduction

In this article we describe some recent results (Finster *et al.* 1999a,b, 2000 a–c, 2002a) concerning the existence of both particle-like, and black hole solutions of the coupled Einstein–Dirac–Yang–Mills (EDYM) equations. We show that there are stable globally defined static, spherically symmetric solutions. We also show that for static black hole solutions, the Dirac wave function must vanish identically outside the event horizon. The latter result indicates that the Dirac particle (fermion) must either enter the black hole or tend to infinity.

The plan of the article is as follows. The next section describes the background material. It is followed by a discussion of the coupled EDYM equations for static, spherically symmetric particle-like and black hole solutions. The final section of the article is devoted to a discussion of these results.

Background Material

Einstein's Equations

We begin by describing the Einstein equation for the gravitational field (for more details, see, e.g., Adler *et al.* (1975)). We first note Einstein's hypotheses of general relativity (GR):

- (E1) The gravitational field is the metric g_{ij} in $3 + 1$ spacetime dimensions. The metric is assumed to be symmetric.
- (E2) At each point in spacetime, the metric can be diagonalized as $\text{diag}(-1, 1, 1, 1)$.
- (E3) The equations which describe the gravitational field should be covariant; that is, independent of the choice of coordinate system.

The hypothesis (E1) is Einstein's brilliant insight, whereby he “geometrizes” the gravitational field. (E2) means that there are inertial frames at each point (but not globally), and guarantees that special relativity (SR) is included in GR, while (E3) implies

that the gravitational field equations must be tensor equations; that is, coordinates are an artifact, and physics should not depend on the choice of coordinates.

Einstein's Equations of GR

The metric $g_{ij} = g_{ij}(x)$, $i, j = 0, 1, 2, 3$, $x = (x^0, x^1, x^2, x^3)$, $x^0 = ct$ (c = speed of light, t = time), is the metric tensor defined on four-dimensional spacetime. Einstein's equations are ten (tensor) equations for the unknown metric g_{ij} (gravitational field), and take the form

$$R_{ij} - \frac{1}{2} R g_{ij} = \sigma T_{ij} \quad [1]$$

where the left-hand side $G_{ij} = R_{ij} - \frac{1}{2} R g_{ij}$ is the Einstein tensor and depends only on the geometry, $\sigma = 8\pi G/c^4$, where G is Newton's gravitational constant, while T_{ij} , the energy–momentum tensor, represents the source of the gravitational field, and encodes the distribution of matter. (The word “matter” in GR refers to everything which can produce a gravitational field, including elementary particles, electromagnetic or Yang–Mills (YM) fields. From the Bianchi identities in geometry (cf. Adler *et al.* (1975)), the (covariant) divergence of the Einstein tensor, G_{ij} , vanishes identically, namely

$$G^j_{i,j} = 0$$

so, on solutions of Einstein's equations,

$$T^j_{i,j} = 0$$

and this in turn expresses the conservation of energy and momentum. The quantities which comprise the Einstein tensor are given as follows: first, from the metric tensor g_{ij} , we form the Levi-Civita connection Γ^k_{ij} defined by:

$$\Gamma^k_{ij} = \frac{1}{2} g^{kl} \left(\frac{\partial g_{lj}}{\partial x^i} + \frac{\partial g_{li}}{\partial x^j} - \frac{\partial g_{ij}}{\partial x^l} \right)$$

where $(4 \times 4 \text{ matrix}) [g^{kl}] = [g_{kl}]^{-1}$, and summation convention is employed; namely, an index which appears as both a subscript and a superscript is to be summed from 0 to 3. With the aid of Γ^k_{ij} , we can

construct the celebrated Riemann curvature tensor R^i_{qkl} :

$$R^i_{qkl} = \frac{\partial \Gamma^i_{ql}}{\partial x^k} - \frac{\partial \Gamma^i_{qk}}{\partial x^l} + \Gamma^i_{pk} \Gamma^p_{ql} - \Gamma^i_{pl} \Gamma^p_{qk}$$

Finally, the terms R_{ij} and R which appear in the Einstein tensor G_{ij} are given by

$$R_{ij} = R^s_{isj}$$

(the Ricci tensor), and

$$R = g^{ij} R_{ij}$$

is the scalar curvature.

From the above definitions, one sees at once the enormous complexity of the Einstein equations. For this reason, one usually seeks solutions which have a high degree of symmetry, and in what follows, in this section, we shall only consider static, spherically symmetric solutions; that is, solutions which depend only on $r = |x| = \sqrt{(x^1)^2 + (x^2)^2 + (x^3)^2}$. In this case, the metric g_{ij} takes the form

$$ds^2 = -T(r)^2 dt^2 + A(r)^{-1} dr^2 + r^2 d\Omega^2 \quad [2]$$

where $d\Omega^2 = d\theta^2 + \sin^2 \theta d\varphi^2$ is the standard metric on the unit 2-sphere, r, θ, φ are the usual spherical coordinates, and t denotes time.

Black Hole Solutions

Consider the problem of finding the gravitational field outside a ball of mass M in \mathbb{R}^3 ; that is, there is no matter exterior to the ball. Solving Einstein's equations $G_{ij}' = 0$ gives the famous Schwarzschild solution (1916):

$$ds^2 = - \left(1 - \frac{2m}{r}\right) c^2 dt^2 + \left(1 - \frac{2m}{r}\right)^{-1} dr^2 + r^2 d\Omega^2 \quad [3]$$

where $m = GM/c^2$. Since $2m$ has the dimensions of length, it is called the Schwarzschild radius. Observe that when $r = 2m$, the metric is singular; namely, $g_{tt} = 0$ and $g_{rr} = \infty$. By transforming the metric [2] to the so-called Kruskal coordinates (cf. Adler *et al.* (1975)), one observes that the Schwarzschild sphere $r = 2m$ has the physical characteristics of a black hole: light and nearby particles can enter the region $r < 2m$, nothing can exit this region, and there is an intrinsic (nonremovable) singularity at the center $r = 0$.

For the general metric [2], we define a black hole solution of Einstein's equations to be a solution which satisfies, for some $\rho > 0$,

$$A(\rho) = 0, \quad A(r) > 0 \text{ if } r > \rho$$

ρ is called the radius of the black hole, or the event horizon.

Yang-Mills Equations

The YM equations generalize Maxwell's equations. To see how this comes about, we first write Maxwell's equations in an invariant way. Thus, let A denote a scalar-valued 1-form:

$$A = A_i dx^i, \quad A_i \in \mathbb{R}$$

which is called the electromagnetic potential (by physicists), or a connection (by geometers). The electromagnetic field (curvature) is the 2-form

$$F = dA$$

In local coordinates,

$$F = F_{ij} dx^i \wedge dx^j, \quad F_{ij} = \frac{\partial A_j}{\partial x^i} - \frac{\partial A_i}{\partial x^j}$$

In this framework, Maxwell's equations are given by

$$d^*F = 0, \quad dF = 0 \quad [4]$$

where \star is the Hodge star operator, mapping 2-forms to 2-forms (in \mathbb{R}^4), and is defined by

$$(*F)_{kl} = \frac{1}{2} \sqrt{|g|} \varepsilon_{ijkl} F^{ij}$$

where $g = \det(g_{ij})$ and ε_{ijkl} is the completely anti-symmetric symbol defined by $\varepsilon_{ijkl} = \text{sgn}(ijkl)$. As usual, indices are raised (or lowered) via the metric, so that, for example,

$$F^{ij} = g^{li} g^{mj} F_{lm}$$

It is important to notice that $*F$ depends on the metric. Note also that Maxwell's equations are linear equations for the A_i 's.

The YM equations generalize Maxwell's equations and can be described as follows. With each YM field (described below) is associated a compact Lie group G called the gauge group. For such G , we denote its Lie algebra by \mathfrak{g} , defined to be the tangent space at the identity of G . Now let A be a \mathfrak{g} -valued 1-form

$$A = A_i dx^i$$

where each A_i is in \mathfrak{g} . In this case, the curvature 2-form is defined by

$$F = dA + A \wedge A$$

or, in local coordinates,

$$F_{ij} = \frac{\partial A_j}{\partial x^i} - \frac{\partial A_i}{\partial x^j} + [A_i, A_j]$$

The commutator $[A_i, A_j] = 0$ if G is an abelian group, but is generally nonzero if G is a matrix group. In this framework, the YM equations can be written in the form $d^*F = 0$, where now d is an appropriately defined covariant exterior derivative. For Maxwell's equations, the gauge group $G = U(1)$ (the circle group $\{e^{i\theta} : \theta \in \mathbb{R}\}$) so \mathfrak{g} is abelian and we recover Maxwell's equations from the YM equations. Observe that if G is nonabelian, then the YM equations $d^*F = 0$ are nonlinear equations for the connection coefficients A_i .

The Dirac Equation in Curved Spacetime

The Dirac equation is a generalization of Schrödinger's equation, in a relativistic setting (Bjorken and Drell 1964). It thus combines quantum mechanics with the theory of relativity. In addition, the Dirac equation also describes the intrinsic "spin" of fermions and, for this reason, solutions of the Dirac equation are often called spinors.

The Dirac equation can be written as

$$(G - m)\Psi = 0 \quad [5]$$

where G is the Dirac operator, m is the mass of the Dirac particle (fermion), and Ψ is a complex-valued 4-vector called the wave function, or spinor. The Dirac operator G is of the form

$$G = iG^j(x) \frac{\partial}{\partial x^j} + B(x) \quad [6]$$

where G^j as well as B are 4×4 matrices, m is the (rest) mass of the fermion, and $i = \sqrt{-1}$. The Dirac equation is thus a linear equation for the spinors. The G^j (called Dirac matrices) and the Lorentzian metric g_{ij} are related by

$$g^{jk}I = \frac{1}{2} \{G^j, G^k\} \quad [7]$$

where $\{G^j, G^k\}$ is the anticommutator

$$\{G^j, G^k\} = G^j G^k + G^k G^j$$

Thus, the Dirac matrices depend on the underlying metric in four-dimensional spacetime.

Suppose that H is a spacelike hypersurface in \mathbb{R}^4 , with future-directed normal vector $\nu = \nu(x)$, and let $d\mu$ be the invariant measure on H induced by the metric g_{ij} . We define a scalar product on solutions Ψ, Φ of the Dirac equation by

$$\langle \Psi | \Phi \rangle = \int_H \bar{\Psi} G^j \Phi \nu_j d\mu \quad [8]$$

This scalar product is positive definite, and because of current conservation (cf. Finster (1988))

$$\nabla_j \bar{\Psi} G^j \Phi = 0$$

it is also independent of H . By generalizing the expression (due to Dirac), $\bar{\Psi} \gamma^0 \Psi = |\Psi|^2$, in Minkowski space, where γ^0 and $\bar{\Psi}$, the adjoint spinors, are defined by

$$\gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \bar{\Psi} = \Psi^* \gamma^0$$

where $*$ denotes complex conjugation, and 1 is the 2×2 identity matrix, the quantity $\bar{\Psi} G^j \Psi \nu_j$ is interpreted as the probability density of the Dirac particle. We normalize solutions of the Dirac equation by requiring

$$\langle \Psi | \Psi \rangle = 1 \quad [9]$$

Spherically Symmetric EDYM Equations

In the remainder of this article we assume that all fields are spherically symmetric, so they depend only on the variable $r = |x|$. In this case, the Lorentzian metric in polar coordinates (t, r, θ, φ) takes the form [2]. The Dirac wave function can be (Finster *et al.* 2000b) described by two real functions, $(\alpha(r), \beta(r))$, and the potential $W(r)$ corresponds to the magnetic component of an $SU(2)$ YM field. As shown in Finster *et al.* (2000b), the EDYM equations are

$$\sqrt{A} \alpha' = \frac{w}{r} \alpha - (m + \omega T) \beta \quad [10]$$

$$\sqrt{A} \beta' = (-m + \omega T) \alpha - \frac{w}{r} \beta \quad [11]$$

$$rA' = 1 - A - \frac{1}{e^2} \frac{(1 - w^2)^2}{r^2} - 2\omega T^2(\alpha^2 + \beta^2) - \frac{2}{e^2} A w'^2 \quad [12]$$

$$2rA' \frac{T'}{T} = -1 + A + \frac{1}{e^2} \frac{(1 - w^2)^2}{r^2} + 2mT(\alpha^2 - \beta^2) - 2\omega T^2(\alpha^2 + \beta^2) + 4 \frac{T}{r} w \alpha \beta - \frac{2}{e^2} A w'^2 \quad [13]$$

$$rA w'' = -(1 - w^2)w + e^2 r T \alpha \beta - r^2 \frac{A'T - 2AT'}{2T} w' \quad [14]$$

Equations [10] and [11] are the Dirac equations, [12] and [13] are the Einstein equations, and [14] is

the YM equation. The constants m, ω , and e denote, respectively, the rest mass of the Dirac particle, its energy, and the YM coupling constant.

Nonexistence of Black Hole Solutions

Let the surface $r = \rho > 0$ represent a black hole event horizon:

$$A(\rho) = 0, \quad A(r) > 0 \text{ if } r > \rho \quad [15]$$

In this case, the normalization condition [9] is replaced by

$$\int_{r_0}^{\infty} (\alpha^2 + \beta^2) \frac{\sqrt{T}}{A} dr < \infty, \quad \text{for every } r_0 > \rho \quad [16]$$

In addition, we assume that the following global conditions hold:

$$\lim_{r \rightarrow \infty} r(1 - A(r)) = M < \infty \quad [17]$$

(finite mass),

$$\lim_{r \rightarrow \infty} T(r) = 1 \quad [18]$$

(gravitational field is asymptotically flat Minkowskian), and

$$\lim_{r \rightarrow \infty} (w(r)^2, w'(r)) = (1, 0) \quad [19]$$

(the YM field is well behaved).

Concerning the event horizon $r = \rho$, we make the following regularity assumptions:

1. The volume element $\sqrt{|\det g_{ij}|} = |\sin \theta| r^2 A^{-1} T^{-2}$ is smooth and nonzero on the horizon; that is,

$$T^{-2} A^{-1}, T^2 A \in C^1([\rho, \infty))$$

2. The strength of the YM field F_{ij} is given by

$$\text{tr}(F_{ij} F^{ij}) = \frac{2Aw^2}{r^4} + \frac{(1 - w^2)^2}{r^4}$$

(cf. Bartnik and McKinnon 1988). We assume that this scalar is bounded near the horizon; that is, outside the event horizon and near $r = \rho$, assume that

$$w \text{ and } Aw^{/2} \text{ are bounded} \quad [20]$$

3. The function $A(r)$ is monotone increasing outside of and near the event horizon.

As discussed in Finster *et al.* (1999a), if assumption 1 or 2 were violated, then an observer freely falling into the black hole would feel strong forces when

crossing the horizon. Assumption 3 is considerably weaker than the corresponding assumption in Finster *et al.* (1999b), where, indeed, it was assumed that the function $A(r)$ obeyed a power law $A(r) = c(r - \rho)^s + \mathcal{O}((r - \rho)^{s+1})$, with positive constants c and s , for $r > \rho$.

The main result in this subsection is the following theorem:

Theorem 1 *Every black hole solution of the EDYM equations [10]–[14] satisfying the regularity conditions 1–3 cannot be normalized and coincides with a Bartnik–McKinnon (BM) black hole of the corresponding Einstein–Yang–Mills (EYM) equations; that is, the spinors α and β must vanish identically outside the event horizon.*

Remark Smoller and Wasserman (1998) proved that any black hole solution of the EYM equations that has finite mass (i.e., that satisfies [17]) must be one of the BM black hole solutions (Bartnik and McKinnon 1988) whose existence was first demonstrated in Smoller *et al.* (1993). Thus, amending the EYM equations by taking quantum-mechanical effects into account – in the sense that both the gravitational and YM fields can interact with Dirac particles – does not yield any new types of black hole solutions.

The present strategy in proving this theorem is to assume that we have a black hole solution of the EDYM equations [10]–[18] satisfying assumptions 1–3, where the spinors do not vanish identically outside of the black hole. We shall show that this leads to a contradiction. The proof is broken up into two cases: either $A^{-1/2}$ is integrable or nonintegrable near the event horizon. We shall only discuss the proof for the case when $A^{-1/2}$ is integrable near the event horizon, leaving the alternate case for the reader to view in Finster *et al.* (2000a).

If $A^{-1/2}$ is integrable, then one shows that there are positive constants c, ε such that

$$c \leq \alpha^2(r) + \beta^2(r) \leq \frac{1}{c}, \quad \text{if } \rho < r < \rho + \varepsilon \quad [21]$$

Indeed, multiplying [10] by α , and [11] by β and adding gives an estimate of the form

$$\sqrt{A}(\alpha^2 + \beta^2)' \leq \kappa(\alpha^2 + \beta^2)$$

Upon dividing by $\sqrt{A}(\alpha^2 + \beta^2)$ and integrating from $r > \rho$ to $\rho + \varepsilon$ gives

$$|\log(\alpha^2 + \beta^2)(\rho + \varepsilon) - \log(\alpha^2 + \beta^2)(r)| \leq \text{const.}$$

from which the desired result follows. Next, from [12] and [13],

$$\begin{aligned} r(AT^2)' &= 4 - \omega T^4(\alpha^2 + \beta^2) \\ &\quad + T^3 \left[2m(\alpha^2 - \beta^2) + \frac{4w}{r}\alpha\beta \right] \\ &\quad - \frac{4}{e^2}(Aw')^2 T^2 \end{aligned} \quad [22]$$

Using assumption 2 together with the last theorem, we see that the coefficients of T^4 , T^3 , and T^2 on the right-hand side of [21] are bounded near ρ , and from assumption 1 the left-hand side of [21] is bounded near ρ . Since assumption 1 implies $T(r) \rightarrow \infty$ as $r \searrow \rho$, we see that $\omega=0$. Since $\omega=0$, the Dirac equations simplify and we can show that $\alpha\beta$ is a positive decreasing function which tends to 0 as $r \rightarrow \infty$. Then the YM equation can be written in the form

$$\begin{aligned} r^2(Aw')' &= -w(1-w)^2 \\ &\quad + e^2 \frac{r(T\sqrt{A})\alpha\beta}{\sqrt{A}} + r^2 \frac{(AT^2)'}{2AT^2} (Aw') \end{aligned} \quad [23]$$

From assumption 2, Aw'^2 is bounded so $A^2w'^2 \rightarrow 0$ as $r \searrow \rho$. Thus, from [22] we can write, for r near ρ ,

$$(Aw')'(r) \geq c_1 + \frac{c_2}{\sqrt{A(r)}}$$

where c_1 and c_2 are positive constants. Using this inequality, we can show that for r near ρ ,

$$A(r) = (r - \rho)B(r)$$

where $0 < \lim_{r \searrow \rho} B(r) < \infty$. It follows that $A(\rho) = 0$ and $A'(\rho) > 0$. Thus, the Einstein metric has the same qualitative features as the Schwarzschild metric near the event horizon. Hence, the metric singularity can be removed via a Kruskal transformation (Adler *et al.* 1975). In these Kruskal coordinates, the YM potential is continuous and bounded (as is easily verified). As a consequence, the arguments in Finster *et al.* (2000c) go through and show that the spinors must vanish identically outside the horizon. For this, one must note that continuous zero-order terms in the Dirac operator are irrelevant for the derivation of the matching conditions in Finster *et al.* 2000c, section 2.4). Thus, the matching conditions (equations (2.31), (2.34) of Finster *et al.* (2000c)) are valid without changes in the presence of our YM field. Using conservation of the (electromagnetic) Dirac current and its positivity in timelike directions, the arguments in Finster *et al.* (2000c, section 4) all carry over. This completes the proof.

We have thus proved that the only black hole solutions of our EDYM equations are the BM black

holes; that is, the spinors must vanish identically. In other words, the EDYM equations do not admit normalizable black hole solutions. Thus, in the presence of quantum-mechanical Dirac particles, static and spherically symmetric black hole solutions do not exist. Another interpretation of these our result is that Dirac particles can only either disappear into the black hole or escape to infinity. These results were proved under very weak regularity assumptions on the form of the event horizon (see assumptions 1–3).

Particle-Like Solutions

By a particle-like (bound state) solution of the (SU(2)) EDYM equations, we mean a smooth solution of eqns [10]–[14], which is defined for all $r \geq 0$, and satisfies condition [9], which explicitly becomes

$$\int_0^r (\alpha^2 + \beta^2) \frac{\sqrt{T}}{A} dr = 1 \quad [24]$$

In addition, we demand that [17]–[19] also hold. It is easily shown that, near $r=0$, we must have

$$w(r) = 1 - \frac{\lambda}{2}r^2 + \mathcal{O}(r^2) \quad [25]$$

where λ is a real parameter. From this, via a Taylor expansion, one finds that

$$\begin{aligned} \alpha(r) &= \alpha_1 r + \mathcal{O}(r^3) \\ \beta(r) &= \frac{1}{2}(\omega T_0 - m)\alpha_1 r^2 + \mathcal{O}(r^3) \end{aligned} \quad [26]$$

$$A(r) = 1 + \mathcal{O}(r^2), \quad T(r) = T_0 + \mathcal{O}(r^2) \quad [27]$$

with two parameters α_1 and $T_0 > 0$. Using linearity of the Dirac equation, we can always assume that $\alpha_1 > 0$.

Under all realistic conditions, the coupling of Dirac particles to the YM field (describing the weak or strong interactions) is much stronger than the coupling to the gravitational field. Thus, we are particularly intrested in the case of weak gravitational coupling. As shown in Finster *et al.* (2000b), the gravitational field is essential for the formation of bound states. However, for arbitrarily weak gravitational coupling, we can hope to find bound states. It is even conceivable that these bound-state solutions might have a well-defined limit when the gravitational coupling tends to zero, if we let the YM coupling go to infinity at the same time. Our idea is that this limiting case might yield a system of equations which is simpler than the full EDYM system, and can thus serve as a physically interesting starting point for the analysis of the coupled

interactions described by the EDYM equations. Expressed in dimensionless quantities, we shall thus consider the limits

$$m^2\kappa \rightarrow 0 \quad \text{and} \quad e^2 \rightarrow \infty \quad [28]$$

That is, we ask whether weak gravitational coupling can give rise to bound states. Using numerical methods, we find particle-like solutions which are stable, even for arbitrarily weak gravitational coupling.

Now assuming that [27] holds (weak gravitational coupling), so that $(A, T) \approx (1, 1)$, then we find that the Dirac equations have a meaningful limit only under the assumptions that α converges and that

$$\begin{aligned} m\beta(r) &\rightarrow \hat{\beta}(r), \quad m^2(T(r) - 1) \rightarrow \varphi \\ m(\omega - m) &\rightarrow E \end{aligned} \quad [29]$$

with two real functions $\hat{\beta}, \varphi$ and a real parameter E . Multiplying [29] with m and taking the limits [28] as well as $A, T \rightarrow 1$, the Dirac equations become

$$\alpha' = \frac{w}{r}\alpha - 2\hat{\beta} \quad [30]$$

$$\hat{\beta}' = (E + \varphi)\alpha - \frac{w}{r}\hat{\beta} \quad [31]$$

We next consider the YM equation [14]. The last term in [14] drops out in the limit of weak gravitational coupling [27]. The second summand converges only under the assumption that

$$\frac{e^2}{m} \rightarrow q \quad [32]$$

with q a real parameter, playing the role of an “effective” coupling constant. Together with [27], this implies that $m \rightarrow \infty$. The YM equations thus have the limit

$$r^2 w'' = -(1 - w)^2 w + q r \alpha \hat{\beta} \quad [33]$$

In order to get a well-defined and nontrivial limit of the Einstein equations [13] and [14], we need to assume that the parameter $m^3\kappa$ has a finite, nonzero limit. Since this parameter has the dimension of inverse length, we can arrange by a scaling of our coordinates that

$$m^3\kappa \rightarrow 1 \quad [34]$$

We differentiate the T -equation [13] with respect to r and substitute [12]. Taking the limits [28] and [33], a straightforward calculation yields the equation

$$r^2 \Delta \varphi = -\alpha^2 \quad [35]$$

where $\Delta = r^{-2} \partial_r (r^2 \partial_r)$ is the radial Laplacian in Euclidean \mathbb{R}^3 . Indeed, this equation can be

regarded as Newton’s equation with the Newtonian potential φ . Thus, the limiting case [34] for the gravitational field corresponds to taking the Newtonian limit. Finally, the normalization condition [16] reduces to

$$\int_0^\infty \alpha(r)^2 dr = 1 \quad [36]$$

The boundary conditions [17]–[19], [24]–[26] are transformed into

$$w(r) = 1 - \frac{\lambda}{2} r^2 + \mathcal{O}(r^3), \quad \lim_{r \rightarrow \infty} w(r) = \pm 1 \quad [37]$$

$$\alpha(r) = \alpha_1 r + \mathcal{O}(r^3), \quad \hat{\beta}(r) = \mathcal{O}(r^3) \quad [38]$$

$$\varphi(r) = \varphi_0 + \mathcal{O}(r^3), \quad \lim_{r \rightarrow \infty} \varphi(r) < \infty \quad [39]$$

with the three parameters λ, α_1 , and φ_0 . We point out that the limiting system contains only one coupling constant q . According to [31] and [33], q is in dimensionless form given by

$$e^2 m^2 \kappa \rightarrow q \quad [40]$$

Hence, in dimensionless quantities, the limit [17] describes the situation where the gravitational coupling goes to zero, while the YM coupling constant goes to infinity like $e^2 \sim (m^2 \kappa)^{-1}$. Therefore, this limiting case is called the reciprocal coupling limit (RCL). The reciprocal coupling system is given by eqns [29], [30], [32], and [34] together with the normalization conditions [35] and the boundary conditions [36]–[38]. According to [28], the parameter E coincides up to a scaling factor with $\omega - m$, and thus has the interpretation as the (properly scaled) energy of the Dirac particle. As in Newtonian mechanics, the potential φ is determined only up to a constant $\mu \in \mathbb{R}$; namely, the reciprocal limit equations are invariant under the transformation

$$\varphi \rightarrow \varphi + \mu, \quad E \rightarrow E - \mu \quad [41]$$

To simplify the connection between the EDYM equations, and the RCL equations, we introduce a parameter ε in such a way that as $\varepsilon \rightarrow 0$, EDYM \rightarrow RCL; namely,

$$\varepsilon = \frac{m^2 \kappa}{e^2}$$

Notice that ε describes the relative strength of gravity versus the YM interaction. For realistic physical situations, the gravitational coupling is weak; namely, $m^2 \kappa \ll 1$, but the YM coupling constant is of order 1: $e^2 \sim 1$. So we investigate the parameter range $\varepsilon \ll 1, q \sim 0$. These form the starting points for the numeric below.

We seek stable bound states for weak gravitational coupling. For this purpose, we consider the total binding energy

$$B = M - m \quad [42]$$

where M is the ADM mass defined by [17] and m is the rest mass of the Dirac particle. B is thus the amount of energy set free when the binding is broken. If $B < 0$, then energy is needed to break up the binding. According to Lee (1987), a solution is stable if $B < 0$. In order to find solutions of the RCL equations with $B < 0$, Lee's treatment and a new two-parameter shooting method (Finster *et al.* 2000b) can be used. Stable solutions of these RCL equations then follow (see Finster *et al.* (2000b) for details).

We now turn to the full EDYM equations. Here are the key steps of our method:

1. Find solutions which are small perturbations of the limiting (RCL) solutions.
2. Trace these solutions by gradually changing the coupling constants.
3. This should yield a one-parameter family of solutions which are "far" from the known limiting solutions.

The point is that we use the RCL solutions as a starting point for numerics, and we "continue" these solutions to solutions of the full EDYM equations.

To be somewhat more specific, we see that if we fix ε and q , we have two parameters:

$$\alpha_1 = \alpha'(0) \quad \text{and} \quad E = \omega - m$$

and two conditions at ∞ :

$$\alpha^2 + \beta^2 \rightarrow 0, \quad w^2 \rightarrow 1$$

We consider the EDYM equations with weaker side conditions

$$\begin{aligned} 0 < \lambda^2 &\equiv \int_0^\infty (\alpha^2 + \beta^2) \frac{\sqrt{T}}{A} dr < \infty \\ 0 < \tau &= \lim_{r \rightarrow \infty} T(r) < \infty \\ \lim_{r \rightarrow \infty} w^2(r) &= 1 \\ \rho &= \lim_{r \rightarrow \infty} r(1 - A(r)) < \infty \end{aligned}$$

Then we rescale these solutions to obtain the true side conditions via the transformations

$$\begin{aligned} \tilde{\alpha}(r) &= \sqrt{\tau} \lambda^{-2} \alpha(\lambda^{-2} r) \\ \tilde{\beta}(r) &= \sqrt{\tau} \lambda^{-2} \beta(\lambda^{-2} r) \\ \tilde{A}(r) &= A(\lambda^{-2} r), \quad \tilde{T}(r) = \tau^{-1} T(\lambda^{-2} r) \\ \tilde{m} &= \lambda^{-2} m, \quad \tilde{\omega} = \tau \lambda^{-2} \omega \\ \tilde{\kappa} &= \lambda^6 \kappa, \quad \tilde{e}^2 = \lambda^2 e^2 \end{aligned}$$

Discussion

In this article we have considered the SU(2) EDYM equations. Our first result shows that the only black hole solutions of these equations are the BM black holes; that is, the spinors must vanish identically outside of the black hole. In other words, the EDYM equations do not admit normalizable black hole solutions. Thus, as mentioned earlier, this result indicates that the Dirac particle either enters the black hole or escapes to infinity. Two recent publications (Finster *et al.* 2002a,b) we consider the Cauchy problem for a massive Dirac equation in a charged, rotating-black-hole geometry (the non-extreme Kerr–Newman black hole), with compactly supported initial data outside the black hole. We prove that, in this case, the probability that the Dirac particle lies in any compact set tends to zero as $t \rightarrow \infty$. This means that the Dirac particle indeed either enters the black hole or tends to infinity. We also show that the wave function decays at a rate $t^{-5/6}$ on any compact set outside of the event horizon.

For particle-like solutions of the SU(2) EDYM equations, we find stable bound states for arbitrarily weak gravitational coupling. This shows that as weak as the gravitational interaction is, it has a regularizing effect on the equations. The stability of particle-like solutions of the EDYM equations is in sharp contrast to the EYM equations, where the particle-like solutions are all unstable (Straumann and Zhou 1990).

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See also: Abelian and Nonabelian Gauge Theories using Differential Forms; Black Hole Mechanics; Bosons and Fermions in External Fields; Dirac Operator and Dirac Field; Einstein Equations: Exact Solutions; Einstein Equations: Initial Value Formulation; Noncommutative Geometry and the Standard Model; Relativistic Wave Equations Including Higher Spin Fields; Symmetry Classes in Random Matrix Theory.

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Dirac Operator and Dirac Field

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Introduction

The Dirac equation arose in the early days of quantum mechanics, inspired by the problem of taking special relativity into account in the quantum mechanical description of a freely moving electron. From the outset, however, Dirac looked for an equation that also accommodated the electron spin and that could be modified to include interaction with an external electromagnetic field. The equation he discovered satisfies all of these requirements. On the other hand, when it is rewritten in Hamiltonian form, the spectrum of the resulting Dirac operator includes not only the desired interval $[mc^2, \infty)$ (where m is the electron mass and c the speed of light), but also an interval $(-\infty, -mc^2]$.

Dirac himself already considered this negative part of the spectrum as unphysical, since no such negative energies had been observed and their presence would entail instability of the electron. This physical flaw of the “first-quantized” description of a relativistic electron led to the introduction of “second quantization,” as encoded in quantum field theory. In the field-theoretic version of the Dirac theory, the unphysical negative energies are obviated by a prescription that originated in Dirac’s hole theory.

Specifically, Dirac postulated that the negative-energy states of his equation were occupied by a sea of unobservable particles, the Pauli principle

forbidding an occupancy greater than one. In this heuristic picture, the annihilation of a negative-energy electron yields a hole in the sea, observable as a new type of positive-energy particle with the same mass, but opposite charge. This led Dirac to predict that the electron should have an oppositely charged partner.

His prediction was soon confirmed experimentally, the partner of the negatively charged electron showing up as the positively charged positron. More generally, all electrically charged particles (not only spin-1/2 particles described by the Dirac equation) have turned out to have oppositely charged antiparticles. Furthermore, some electrically neutral particles also have distinct antiparticles.

Returning to the second-quantized Dirac theory, this involves a Dirac quantum field in which the creation/annihilation operators of negative-energy states are replaced by annihilation/creation operators of positive-energy holes, resp. The hole theory substitution therefore leads to a Hilbert space (called Fock space) that accommodates an arbitrary number of particles and antiparticles with the same mass and opposite charge.

Soon after the introduction of the Dirac equation (which dates from 1928), it turned out that the number of particles and antiparticles is not conserved in a high-energy collision. Such creation and annihilation processes admit a natural description in the Fock spaces associated with relativistic quantum field theories. The very comprehensive mathematical description of real-world elementary particle phenomena that is now called the standard model arose some 30 years ago, and has been abundantly confirmed by experiment ever since. It involves

various relativistic quantum fields with nonlinear interactions. The Dirac quantum field is an essential ingredient, inasmuch as it is used to describe all spin-1/2 particles and antiparticles in the model (including quarks, electrons, neutrinos etc.).

After this survey (which is not only very brief, but also biased toward the physical concepts at issue), the contents of this article will be sketched. The free Dirac equation associated with the physical Minkowski spacetime \mathbb{R}^4 is first detailed. The exposition and notation are slightly unconventional in some respects. This is because we are partly preparing the ground for a mathematically precise account of the second-quantized version of the free Dirac theory. For example, momentum space (as opposed to position space) is emphasized, since the variable x in the Dirac equation does not have a clear physical significance and should be discarded in the Hilbert space formulation of the second-quantized Dirac field. The latter acts on a Fock space of multi-particle and -antiparticle wave functions depending on momentum and spin variables, and the spacetime dependence of the Dirac field is solely a consequence of relativistic covariance. (In particular, the variable x in the Dirac field $\Psi(t, x)$ should not be viewed as the position of particles and antiparticles created and annihilated by the field.)

To be sure, there is much more to the Dirac theory than its free first- and second-quantized versions for Minkowski spacetime \mathbb{R}^4 . The primary purpose here is, however, to present these foundational versions in some detail. A much more sketchy account of further developments can be found in subsequent sections. First, the one-particle theory is reconsidered. Generalizations of the free theory to arbitrary dimensions and Euclidean settings are sketched and interactions with external fields are described, touching on various aspects and applications.

The next focus is on relations with index theory that arise when the massless Euclidean Dirac operator is generalized to geometric settings, namely l -dimensional Riemannian manifolds allowing a spin structure. We illustrate the general Atiyah–Singer index theory for the Dirac framework with some simple examples for $l=1$ (Toeplitz operators) and $l=2$ (the manifold $S^1 \times S^1$).

More information on the many-particle Dirac theory appears in the final section. Brief remarks on the Dirac field in interaction with other quantized fields are followed by an elaboration of the far simpler situation of the Dirac field interacting with external fields. Among the S -operators corresponding to such fields there is a

special class of unitary matrix multipliers; the external field then vanishes for $t < 0$ and equals the pure gauge field corresponding to the unitary matrix for $t \geq 0$. Specializing to an even spacetime dimension and choosing special “kink” type unitaries, the associated Fock-space quadratic forms can be made to converge to the free Dirac field.

As mentioned already, Dirac’s second quantization procedure was invented to get rid of the unphysical negative energies of the first-quantized (one-particle) theory. It is an amazing fact that the resulting formalism for the simplest case (namely the massless Dirac operator in a two-dimensional spacetime) can be exploited for quite different purposes. In particular, this setting can be tied in with various soliton equations and the representation theory of certain infinite-dimensional groups and Lie algebras. In conclusion, some of these applications are briefly sketched, namely the construction of special solutions to the Kadomtsev–Petviashvili (KP) equation (including the KP solitons and finite-gap solutions) and special representations of Kac–Moody and Virasoro algebras.

The Free One-Particle Dirac Equation in \mathbb{R}^4

The free time-dependent Dirac equation is a linear hyperbolic evolution equation for a function $\Psi(t, x)$ on spacetime \mathbb{R}^4 with values in \mathbb{C}^4 . It involves four 4×4 matrices γ^μ , $\mu=0, 1, 2, 3$, satisfying the γ -algebra

$$\gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2g^{\mu\nu} \mathbf{1}_4, \quad g = \text{diag}(1, -1, -1, -1) \quad [1]$$

Using the Pauli matrices

$$\begin{aligned} \sigma_1 &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, & \sigma_2 &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ \sigma_3 &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{aligned} \quad [2]$$

one can choose for example

$$\begin{aligned} \gamma^0 &= \begin{pmatrix} 0 & \mathbf{1}_2 \\ \mathbf{1}_2 & 0 \end{pmatrix}, & \gamma^k &= \begin{pmatrix} 0 & -\sigma_k \\ \sigma_k & 0 \end{pmatrix} \\ k &= 1, 2, 3 \end{aligned} \quad [3]$$

Now the free Dirac equation reads

$$(i\hbar\gamma^0\partial_t + i\hbar c\gamma \cdot \nabla - mc^2\mathbf{1}_4)\Psi(t, x) = 0 \quad [4]$$

where \hbar is Planck's constant, c the speed of light, and m the particle mass. Using from now on units so that $\hbar = c = 1$, this can be abbreviated as

$$\left(i \sum_{\mu=0}^3 \gamma^\mu \partial_\mu - m \right) \Psi(x) = 0, \quad x = (x^0, x^1, x^2, x^3) \quad [5]$$

$$\partial_\mu = \partial / \partial x^\mu, \quad \mu = 0, 1, 2, 3$$

The relativistic invariance of this equation can be understood as follows. First, since the equation does not explicitly involve the spacetime coordinates, it is invariant under spacetime translations. (If $\Psi(t, \mathbf{x})$ solves [5], then also $\Psi(t - a_0, \mathbf{x} - \mathbf{a})$ is a solution for all $(a_0, \mathbf{a}) \in \mathbb{R}^4$.) Second, it is invariant under Lorentz transformations (rotations and boosts). Indeed, if $\Psi(x)$ is a solution and $L \in \text{SO}(1, 3)$, then $S(L)\Psi(L^{-1}x)$ solves [5] too, where $S(L)$ denotes a (suitably normalized) matrix satisfying

$$S(L)^{-1} \gamma^\mu S(L) = \sum_{\nu=0}^3 L^\mu{}_\nu \gamma^\nu \quad [6]$$

(The matrices γ^μ on the right-hand side of [6] satisfy the γ -algebra [1]. From this, the existence of a representation $S(L)$ of $\text{SO}(1, 3)$ satisfying [6] is readily deduced.)

As a consequence, the Poincaré group (inhomogeneous Lorentz group) acts in a natural way on the space of solutions to the time-dependent Dirac equation, expressing its independence of the choice of inertial frame. For quantum mechanical purposes, however, one needs to choose a frame and use the associated time variable to rewrite the equation as a Hilbert space evolution equation.

The relevant Hilbert space $\check{\mathcal{H}}$ is the space of four-component functions that are square integrable over space,

$$\check{\mathcal{H}} = L^2(\mathbb{R}^3, d\mathbf{x}) \otimes \mathbb{C}^4 \quad [7]$$

To obtain a self-adjoint Hamiltonian on $\check{\mathcal{H}}$, one multiplies [5] by γ^0 and introduces the Hermitian matrices

$$\beta = \gamma^0, \quad \alpha^k = \gamma^0 \gamma^k, \quad k = 1, 2, 3 \quad [8]$$

Then, one obtains the Schrödinger type equation

$$i \frac{d}{dt} \psi = \check{H} \psi \quad [9]$$

where \check{H} is the Dirac operator,

$$\check{H} = -i\alpha \cdot \nabla + \beta m \quad [10]$$

Under Fourier transformation,

$$\mathcal{F}: \check{\mathcal{H}} \rightarrow L^2(\mathbb{R}^3, d\mathbf{p}) \otimes \mathbb{C}^4$$

$$\psi(\mathbf{x}) \mapsto \phi(\mathbf{p}) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} d\mathbf{x} \exp(-i\mathbf{x} \cdot \mathbf{p}) \psi(\mathbf{x}) \quad [11]$$

eqn [9] turns into

$$i \frac{d}{dt} \phi = D(\mathbf{p}) \phi, \quad D(\mathbf{p}) = \alpha \cdot \mathbf{p} + \beta m \quad [12]$$

The matrix $D(\mathbf{p})$ is Hermitian and has square $E_p^2 \mathbf{1}_4$, where E_p is the relativistic energy,

$$E_p = (\mathbf{p} \cdot \mathbf{p} + m^2)^{1/2} \quad [13]$$

corresponding to a momentum \mathbf{p} . Now, we have

$$U_C \overline{D(-\mathbf{p})} = -D(\mathbf{p}) U_C \quad [14]$$

where U_C is the charge conjugation matrix,

$$U_C = i\gamma^2 \quad [15]$$

Hence, the four eigenvalues of $D(\mathbf{p})$ are given by $E_p, E_p, -E_p$, and $-E_p$. Therefore, the matrices

$$P_\pm(\mathbf{p}) = \frac{1}{2} \left(\mathbf{1}_4 \pm \frac{D(\mathbf{p})}{E_p} \right) \quad [16]$$

are projections on the positive and negative spectral subspaces of $D(\mathbf{p})$.

As orthonormal base for the positive-energy subspace, we can now choose

$$w_{+,j}(\mathbf{p}) = \left(\frac{2E_p}{E_p + m} \right)^{1/2} P_+(\mathbf{p}) b_j, \quad j = 1, 2 \quad [17]$$

where

$$b_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad b_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix} \quad [18]$$

Next, setting

$$w_{-,j}(\mathbf{p}) = U_C \overline{w_{+,j}(\mathbf{p})}, \quad j = 1, 2 \quad [19]$$

an orthonormal base $w_{-,1}(-\mathbf{p}), w_{-,2}(-\mathbf{p})$ for the negative-energy subspace of $D(\mathbf{p})$ is obtained; cf. [14].

The upshot is that the time-independent Dirac equation

$$\check{H} \psi = E \psi \quad [20]$$

gives rise to bounded eigenfunctions

$$\begin{aligned} e_{+,j}(\mathbf{x}, \mathbf{p}) &= (2\pi)^{-3/2} \exp(i\mathbf{x} \cdot \mathbf{p}) w_{+,j}(\mathbf{p}), \quad j = 1, 2 \\ e_{-,j}(\mathbf{x}, \mathbf{p}) &= (2\pi)^{-3/2} \exp(-i\mathbf{x} \cdot \mathbf{p}) w_{-,j}(\mathbf{p}), \quad j = 1, 2 \end{aligned} \quad [21]$$

with eigenvalues $E = E_p$ and $E = -E_p$, resp. Clearly, they are not square-integrable, but they can be used as the kernel of a unitary transformation between $\check{\mathcal{H}}$ (7) and the Hilbert space

$$\begin{aligned} \mathcal{H} &= \mathcal{H}_+ \oplus \mathcal{H}_- = P_+ \mathcal{H} \oplus P_- \mathcal{H} \\ \mathcal{H}_+, \mathcal{H}_- &= L^2(\mathbb{R}^3, d\mathbf{p}) \otimes \mathbb{C}^2 \end{aligned} \quad [22]$$

Specifically, we have

$$\begin{aligned} W: \mathcal{H} &\rightarrow \check{\mathcal{H}} \\ f(\mathbf{p}) &= (f_+(\mathbf{p}), f_-(\mathbf{p})) \\ \mapsto \psi(\mathbf{x}) &= \sum_{\delta=+,-} \sum_{j=1,2} \int_{\mathbb{R}^3} d\mathbf{p} e_{\delta,j}(\mathbf{x}, \mathbf{p}) f_{\delta,j}(\mathbf{p}) \end{aligned} \quad [23]$$

which entails

$$(W^{-1}\psi)_{\delta,j}(\mathbf{p}) = \int_{\mathbb{R}^3} d\mathbf{x} \bar{e}_{\delta,j}(\mathbf{x}, \mathbf{p}) \cdot \psi(\mathbf{x}) \quad [24]$$

(Here and throughout this article, a bar denotes complex conjugation.)

From the above, it is clear that the Dirac Hamiltonian \check{H} acting on the Hilbert space $\check{\mathcal{H}}$ is unitarily equivalent to the multiplication operator on \mathcal{H} [22] given by

$$(Hf)_{\delta}(\mathbf{p}) = \delta E_p f_{\delta}(\mathbf{p}), \quad \delta = +, - \quad [25]$$

Indeed, W is a diagonalizing transformation for \check{H} , the relation

$$H = W^{-1} \check{H} W \quad [26]$$

yielding an explicit realization of the spectral theorem.

Using the same notational convention, the momentum, charge conjugation, parity, and time-reversal operators on $\check{\mathcal{H}}$, given by

$$(\check{P}_k \psi)(\mathbf{x}) = -i \partial_k \psi(\mathbf{x}) \quad [27]$$

$$(\check{C} \psi)(\mathbf{x}) = U_C \bar{\psi}(\mathbf{x}) \quad [28]$$

$$(\check{P} \psi)(\mathbf{x}) = U_P \psi(-\mathbf{x}), \quad U_P = \gamma^0 \quad [29]$$

$$(\check{T} \psi)(\mathbf{x}) = U_T \bar{\psi}(\mathbf{x}), \quad U_T = \gamma^1 \gamma^3 \quad [30]$$

transform into the operators

$$(P_k f)_{\delta}(\mathbf{p}) = \delta p_k f_{\delta}(\mathbf{p}), \quad \delta = +, - \quad [31]$$

$$(Cf)_{\delta}(\mathbf{p}) = \bar{f}_{-\delta}(\mathbf{p}), \quad \delta = +, - \quad [32]$$

$$(Pf)_{\delta}(\mathbf{p}) = \delta f_{\delta}(-\mathbf{p}), \quad \delta = +, - \quad [33]$$

$$(Tf)_{\delta}(\mathbf{p}) = i\sigma_2 \bar{f}_{\delta}(-\mathbf{p}), \quad \delta = +, - \quad [34]$$

Note that P_k , P , and T leave the positive- and negative-energy subspaces \mathcal{H}_+ and \mathcal{H}_- invariant, whereas C interchanges them.

To conclude this section, we describe some salient features of the unitary representation of the (identity component of the) Poincaré group on \mathcal{H} , which follows from the representation on solutions to [5] already sketched. The spacetime translations over $a \in \mathbb{R}^4$ are represented by the unitary operator $\exp(-ia_0 H + i\mathbf{a} \cdot \mathbf{P})$; explicitly,

$$\begin{aligned} (\exp(-ia_0 H + i\mathbf{a} \cdot \mathbf{P})f)_{\delta}(\mathbf{p}) &= \exp(-i\delta(a_0 E_p - \mathbf{a} \cdot \mathbf{p})) f_{\delta}(\mathbf{p}), \quad \delta = +, - \end{aligned} \quad [35]$$

The representation of the Lorentz group involves unitary 2×2 matrices $U(k, A)$, where k is an arbitrary 4-vector satisfying $k^\mu k_\mu = 1$ and A the matrix in $\text{SL}(2, \mathbb{C})$ representing $L \in \text{SO}(1, 3)$. (Recall that $\text{SL}(2, \mathbb{C})$ can be viewed as a 2-fold cover of $\text{SO}(1, 3)$.) In particular, $U(k, A)$ does not depend on k for rotations,

$$U(k, A) = A^*, \quad \forall A \in \text{SU}(2) \quad [36]$$

(Here and henceforth, we use $*$ to denote the Hermitian adjoint of matrices and operators.) For boosts, however, there is dependence on the vector k , which is the image of the vector $(1, 0)$ under the boost. We refrain from a more detailed description of $U(k, A)$, as this would carry us too far afield.

The unitary $\text{SO}(1, 3)$ representation leaves the decomposition $\mathcal{H} = P_+ \mathcal{H} \oplus P_- \mathcal{H}$ invariant. On the positive-energy subspace \mathcal{H}_+ , it is given by

$$(U(L)f)_+(\mathbf{p}) = \left(\frac{p_0^L}{p_0}\right)^{1/2} U\left(\frac{\mathbf{p}}{m}, A\right)^* f_+(\mathbf{p}^L) \quad [37]$$

where

$$\mathbf{p} = (E_p, \mathbf{p}), \quad \mathbf{p}^L = L^{-1} \mathbf{p} \quad [38]$$

On \mathcal{H}_- , it is given by the complex-conjugate representation,

$$(U(L)f)_-(\mathbf{p}) = \left(\frac{p_0^L}{p_0}\right)^{1/2} U\left(\frac{\mathbf{p}}{m}, A\right)^t \bar{f}_-(\mathbf{p}^L) \quad [39]$$

just as for the spacetime translations, cf. [35]. (The superscript t is used to denote the transpose matrix.) This feature is crucial for the second-quantized Dirac theory, which is discussed next.

The Free Dirac Field in \mathbb{R}^4

The free Dirac field is an operator-valued distribution on a Fock space that describes an arbitrary number of spin-1/2 particles and antiparticles in terms of momentum space wave functions. Since spin-1/2 particles are fermions (which encodes the Pauli exclusion principle), an M -particle wave function $F_{j_1, \dots, j_M}^{+, \dots, +}(p_1, \dots, p_M)$ (where $j_l \in \{1, 2\}$ is the spin index) is antisymmetric under any interchange of a pair (j_i, p_i) and (j_k, p_k) . Likewise, N -antiparticle wave functions $F_{k_1, \dots, k_N}^{-, \dots, -}(q_1, \dots, q_N)$ are antisymmetric. But a wave function $F_{j,k}^{+-}(p, q)$ describing a particle-antiparticle pair need not have any symmetry property, since a particle and an antiparticle can be distinguished by their charge.

The relevant Fock space is therefore the tensor product of two antisymmetric Fock spaces built over the one-particle and one-antiparticle spaces $L^2(\mathbb{R}^3, d\mathbf{p}) \otimes \mathbb{C}^2$. For later purposes, it is important to view these spaces as the summands \mathcal{H}_+ and \mathcal{H}_- of the space \mathcal{H} from the previous section. Thus, the arena for the free Dirac field is the Hilbert space

$$\mathcal{F}_a(\mathcal{H}) \simeq \mathcal{F}_a(\mathcal{H}_+) \otimes \mathcal{F}_a(\mathcal{H}_-) \quad [40]$$

where, for example,

$$\mathcal{F}_a(\mathcal{H}) = (\mathbb{C} \oplus \mathcal{H} \oplus (\mathcal{H} \otimes \mathcal{H})_a \oplus \dots)^- \quad [41]$$

where the bar denotes the completion of the infinite direct sum in the obvious inner product. The tensor $(1, 0, 0, \dots)$ is viewed as the vacuum (the “filled Dirac sea”) and denoted by Ω .

To get around in Fock space, one employs the creation and annihilation operators $c^{(*)}(f)$, $f \in \mathcal{H}$. The creation operator $c^*(f)$, $f \in \mathcal{H}$, is defined by linear and continuous extension of its action on the vacuum Ω and on elementary antisymmetric tensors, recursively given by

$$\begin{aligned} c^*(f)\Omega &= f, \quad c^*(f)f_1 = f \wedge f_1, \dots \\ c^*(f)f_1 \wedge \dots \wedge f_N &= f \wedge f_1 \wedge \dots \wedge f_N, \dots \end{aligned} \quad [42]$$

Its adjoint, the annihilation operator $c(f)$, satisfies

$$\begin{aligned} c(f)\Omega &= 0, \quad c(f)f_1 = (f, f_1)\Omega, \dots \\ c(f)f_1 \wedge \dots \wedge f_N &= \sum_{j=1}^N (-)^{j-1} (f, f_j) \\ &\quad \times f_1 \wedge \dots \wedge \widehat{f_j} \wedge \dots \wedge f_N, \dots \end{aligned} \quad [43]$$

Accordingly, the operators $c^{(*)}(f)$ satisfy the canonical anticommutation relations (CARs) over \mathcal{H} ,

$$\begin{aligned} \{c(f), c(g)\} &= 0, \\ \{c(f), c^*(g)\} &= (f, g), \quad \forall f, g \in \mathcal{H} \end{aligned} \quad [44]$$

where $\{A, B\}$ denotes the anticommutator $AB + BA$. (From this, one readily deduces that $c^{(*)}(f)$ is bounded with norm $\|f\|$.)

Next, recalling the direct sum decomposition [22], a notation change

$$c^{(*)}(P_+f) \rightarrow a^{(*)}(P_+f), \quad c^{(*)}(P_-f) \rightarrow b^{(*)}(P_-f) \quad [45]$$

is made, thus indicating that $a^{(*)}$ and $b^{(*)}$ should be viewed as the creation/annihilation operators of particles and antiparticles, resp. Since \mathcal{H}_+ and \mathcal{H}_- are copies of $L^2(\mathbb{R}^3, d\mathbf{p}) \otimes \mathbb{C}^2$, a given function $(f_1(\mathbf{p}), f_2(\mathbf{p}))$ in the latter space can occur both as an argument of $a^{(*)}(\cdot)$ and of $b^{(*)}(\cdot)$; it can also be viewed as a smearing function for unsmeared quantities $a_j^{(*)}(\mathbf{p})$ and $b_j^{(*)}(\mathbf{p})$, $j=1, 2$, that are often referred to as operators as well (even though they are only quadratic forms). Thus, one has, for example,

$$\begin{aligned} b^*(f) &= \sum_{j=1}^2 \int_{\mathbb{R}^3} d\mathbf{p} b_j^*(\mathbf{p}) f_j(\mathbf{p}) \\ b(f) &= \sum_{j=1}^2 \int_{\mathbb{R}^3} d\mathbf{p} b_j(\mathbf{p}) \bar{f}_j(\mathbf{p}) \end{aligned} \quad [46]$$

As explained shortly, the smeared time-zero Dirac field takes the form

$$\Phi(f) = a(P_+f) + b^*(KP_-f), \quad f \in \mathcal{H} \quad [47]$$

Here and below, K denotes complex conjugation on \mathcal{H} , \mathcal{H}_+ , and \mathcal{H}_- . Just as the operators $c^{(*)}(f)$, the operators $\Phi^{(*)}(f)$ satisfy the CARs over \mathcal{H} ,

$$\begin{aligned} \{\Phi(f), \Phi(g)\} &= 0 \\ \{\Phi(f), \Phi^*(g)\} &= (f, g), \quad \forall f, g \in \mathcal{H} \end{aligned} \quad [48]$$

as is readily verified using [44]–[45]. But this Φ -representation is not unitarily equivalent to the c -representation [44]. This becomes clear in particular from the consideration of a crucial type of CAR automorphism that is considered next.

To this end, we fix a unitary operator U on \mathcal{H} . Then it is plain that the operators

$$\tilde{c}^{(*)}(f) = c^{(*)}(Uf) \quad [49]$$

$$\tilde{\Phi}^{(*)}(f) = \Phi^{(*)}(Uf) \quad [50]$$

also satisfy the CARs. The CAR-algebra automorphism $c^{(*)}(f) \mapsto \tilde{c}^{(*)}(f)$ can be unitarily implemented in $\mathcal{F}_a(\mathcal{H})$, since one has

$$\tilde{c}^{(*)}(f) = \Gamma(U)c^{(*)}(f)\Gamma(U^*) \quad [51]$$

where $\Gamma(U)$ denotes the Fock-space product operator corresponding to U . Thus, for example,

$$\begin{aligned} \Gamma(U)\Omega &= \Omega, \quad \Gamma(U)f = Uf, \dots \\ \Gamma(U)f_1 \wedge \dots \wedge f_N &= Uf_1 \wedge \dots \wedge Uf_N, \dots \end{aligned} \quad [52]$$

For the CAR automorphism $\Phi^{(*)}(f) \mapsto \tilde{\Phi}^{(*)}(f)$ this is not true, however. Rewriting it in terms of the annihilation and creation operators $a^{(*)}$ and $b^{(*)}$ via [47], it amounts to a linear transformation (Bogoliubov transformation), whose unitary implementability has been clarified several decades ago. To be specific, the necessary and sufficient condition for unitary implementability is that the off-diagonal parts

$$U_{+-} = P_+ U P_-, \quad U_{-+} = P_- U P_+ \quad [53]$$

in the 2×2 matrix decomposition of operators on \mathcal{H} be Hilbert-Schmidt operators. Therefore, no problem arises when U is diagonal with respect to this decomposition. Indeed, in that case one can choose as unitary implementer the product operator

$$\tilde{\Gamma}(U) = \Gamma(U_{++}) \otimes \Gamma(KU_{--}K) \quad [54]$$

(cf. the tensor product structure [40] of $\mathcal{F}_a(\mathcal{H})$).

In particular, the automorphism

$$\Phi(f) \mapsto \Phi(e^{itH}f) \quad [55]$$

where H is the free diagonalized Dirac Hamiltonian [25], is implemented by the operator

$$\tilde{\Gamma}(e^{itH}) = \Gamma(e^{itE}) \otimes \Gamma(e^{itE}) \quad [56]$$

where E denotes multiplication by E_p on \mathcal{H}_+ and \mathcal{H}_- . The change of CAR representation, therefore, entails that the unphysical negative energies of the one-particle theory are replaced by positive energies of antiparticles. Hence, we obtain a mathematically precise version of Dirac's hole theory substitution $b_j(p) \rightarrow b_j^*(p)$, $b_j^*(p) \rightarrow b_j(p)$.

More generally, if one chooses for U the Poincaré group representation (given by [35] and [37]–[39]), then the Fock-space implementer [54] is the tensor product of two product operators with the same action on $\mathcal{F}_a(L^2(\mathbb{R}^3, d\mathbf{p}) \otimes \mathbb{C}^2)$. Observe that this is also true for the Fock-space version $\tilde{\Gamma}(T) = \Gamma(T)$ of the time-reversal operator [34]. By contrast, the Fock-space parity operator $\tilde{\Gamma}(P) = \Gamma(P)$ gives rise to two product operators with slightly different actions, cf. [33]. Accordingly, particles and antiparticles have opposite parity.

The map

$$\Phi(f) \mapsto \Phi(Cf)^* \quad [57]$$

also yields a CAR automorphism. It is unitarily implemented by the Fock-space charge-conjugation operator

$$C = \Gamma\left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\right) \quad [58]$$

which interchanges particles and antiparticles. Notice that C is unitary, whereas C is antiunitary.

It remains to establish the precise relation of the above to the customary free Dirac field $\Psi(t, \mathbf{x})$. This is a quadratic form on $\mathcal{F}_a(\mathcal{H})$ given by

$$\begin{aligned} \Psi(t, \mathbf{x}) &= (2\pi)^{-3/2} \int_{\mathbb{R}^3} d\mathbf{p} \sum_{j=1,2} \left(a_j(\mathbf{p}) w_{+j}(\mathbf{p}) e^{-iE_p t + i\mathbf{p} \cdot \mathbf{x}} \right. \\ &\quad \left. + b_j^*(\mathbf{p}) w_{-j}(\mathbf{p}) e^{iE_p t - i\mathbf{p} \cdot \mathbf{x}} \right) \end{aligned} \quad [59]$$

(Its expectation $\langle F_1, \Psi(t, \mathbf{x}) F_2 \rangle$ is, for example, well defined for F_1, F_2 in the dense subspace of $\mathcal{F}_a(\mathcal{H})$ that consists of vectors with finitely many particles and antiparticles and wave functions in Schwartz space.) It satisfies the time-dependent Dirac equation

$$i\partial_t \Psi = (-i\alpha \cdot \nabla + \beta m) \Psi \quad [60]$$

in the sense of quadratic forms. Furthermore, smearing it with a function $\bar{\psi}(\mathbf{x})$ in the Hilbert space $\tilde{\mathcal{H}}$ (7), we obtain

$$\begin{aligned} &\int_{\mathbb{R}^3} d\mathbf{x} \bar{\psi}(\mathbf{x}) \cdot \Psi(t, \mathbf{x}) \\ &= \Phi(e^{itH} W^{-1} \psi) \\ &= \tilde{\Gamma}(e^{itH}) \Phi(W^{-1} \psi) \tilde{\Gamma}(e^{-itH}) \quad \psi \in \tilde{\mathcal{H}} \end{aligned} \quad [61]$$

As announced, the time evolution of the free Dirac field is, therefore, given by the unitary one-parameter group [56], whose generator (the second-quantized Dirac Hamiltonian) has spectrum $\{0\} \cup [m, \infty)$.

The Dirac field $\Psi(t, \mathbf{x})$ can also be smeared with a test function $F(t, \mathbf{x})$ in the Schwartz space $S(\mathbb{R}^4)^4$, yielding a bounded operator

$$\Psi(F) = \int_{\mathbb{R}^4} d\mathbf{x} F(\mathbf{x}) \cdot \Psi(\mathbf{x}) \quad [62]$$

Then one obtains the relativistic covariance relation

$$\tilde{\Gamma}(U(a, L)) \Psi(F) \tilde{\Gamma}(U(a, L))^* = \Psi(F^{a,L}) \quad [63]$$

where

$$F^{a,L}(\mathbf{x}) = S(L^{-1})^t F(L^{-1}(\mathbf{x} - a)) \quad [64]$$

and $U(a, L)$ denotes the Poincaré group representation on \mathcal{H} , cf. [35] and [37]–[39]. Likewise, one gets the inversion formulas

$$\tilde{\Gamma}(I)\Psi(F)\tilde{\Gamma}(I)^* = \Psi(F_I), \quad I = P, T \quad [65]$$

with

$$F_P(t, \mathbf{x}) = U_P^t F(t, -\mathbf{x}), \quad F_T(t, \mathbf{x}) = U_T^t \bar{F}(-t, \mathbf{x}) \quad [66]$$

while the Fock-space charge-conjugation operator [58] transforms the Dirac field as

$$\mathcal{C}\Psi(F)\mathcal{C} = \Psi(F_C)^* \quad [67]$$

with

$$F_C(\mathbf{x}) = U_C^t \bar{F}(\mathbf{x}) \quad [68]$$

Finally, let us consider the global $U(1)$ gauge transformations $f \mapsto e^{i\phi} f$, where $\phi \in \mathbb{R}$ and $f \in \mathcal{H}$. They can be implemented by

$$\tilde{\Gamma}(e^{i\phi}) = \Gamma(e^{i\phi}) \otimes \Gamma(e^{-i\phi}) \quad [69]$$

and one has

$$\tilde{\Gamma}(e^{i\phi})\Psi(F)\tilde{\Gamma}(e^{i\phi})^* = \Psi(F_\phi) \quad [70]$$

with

$$F_\phi(\mathbf{x}) = e^{-i\phi} F(\mathbf{x}) \quad [71]$$

The generator Q of the one-parameter group $\phi \mapsto \tilde{\Gamma}(e^{i\phi})$ is the charge operator: on wave functions describing N_+ particles and N_- antiparticles, it has eigenvalue $N_+ - N_-$.

More on the One-Particle Dirac Theory

Even for the free one-particle setting, the account given earlier is far from complete. To begin with, the free Dirac equation admits a specialization to massless particles. In the Weyl representation of the γ -algebra adopted above, the choice $m=0$ entails that the \mathbf{p} -space equation [12] decouples into two 2×2 equations for spinors that can be labeled by their chirality (“handedness”). This refers to their eigenvalue with respect to the chirality matrix

$$\gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3 = \begin{pmatrix} 1_2 & 0 \\ 0 & -1_2 \end{pmatrix} \quad [72]$$

and this notion derives from the noninvariance of the separate 2×2 equations under parity. (A positive-chirality spinor is mapped to a negative-chirality spinor under the parity operator \check{P} (33) and vice versa.) Since the weak interaction breaks parity symmetry, the two 2×2 equations (often called Weyl equations) do have physical relevance. Indeed,

the associated quantum fields are a crucial ingredient of the standard model.

Next, we point out that it is possible to switch to a representation in which the gamma matrices are real. This so-called Majorana representation is convenient (but not indispensable) in the description of neutral spin-1/2 particles. By definition, such particles are equal to their antiparticles, so that the second-quantized formalism of the previous section must be adapted: one needs the neutral CAR algebra over \mathcal{H} (also known as self-dual CAR).

For various purposes, it is important to formulate the free Dirac equation for a spacetime whose spatial dimension is arbitrary. Then one needs, first of all, gamma matrices satisfying the (Minkowski) Clifford algebra relations

$$\gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2g^{\mu\nu} \mathbf{1}_\Lambda, \quad g = \text{diag}(1, -1_n) \quad [73]$$

where n is the space dimension and the minimal size $\Lambda \times \Lambda$ of the gamma matrices is to be determined.

Clearly, for $n=1$ and $n=2$, one can take $\Lambda=2$, choosing, for example,

$$\begin{aligned} \gamma^0 &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, & \gamma^1 &= \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \\ \gamma^2 &= \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} \end{aligned} \quad [74]$$

to fulfill [73]. For $n=4$, one can take $\Lambda=4$, just as for $n=3$, supplementing [1] with the matrix $i\gamma^5$, cf. [72].

More generally, for $n=2N-1$ and $n=2N$, one can take $\Lambda=2^N$ in [73]. Indeed, a representation on the 2^N -dimensional fermion Fock space $\mathcal{F}_a(\mathbb{C}^N)$ (cf. [41]) is readily constructed using the creation and annihilation operators described in the previous section. Once this has been taken care of, most of the discussion on the free one-particle Dirac equation in \mathbb{R}^4 can be easily generalized. Of special importance in this regard is the straightforward adaptation of the formulas [7]–[26], which form the foundation for the second-quantized version. Indeed, the discussion of the last section applies nearly verbatim for arbitrary spacetime dimension.

In several applications, the so-called Euclidean version of the free Dirac theory in spacetime dimension $n+1$ is important. Basically, this version is obtained upon replacing $i\partial_0$ by ∂_{n+1} in the Dirac equation, a substitution that changes the character of the equation from hyperbolic to elliptic. Provided that the mass vanishes, the Euclidean Dirac equation admits a reinterpretation as a time-independent zero-eigenvalue Weyl equation in a Minkowski spacetime of dimension $n+2$. (This equation is often called the zero-mode equation.)

Let us now turn to the description of the interaction with an external electromagnetic potential $A_\mu(t, \mathbf{x})$. This can be taken into account via the minimal substitution,

$$\partial_\mu \rightarrow \partial_\mu + ieA_\mu \quad [75]$$

also known as the covariant derivative, in the time-dependent Dirac equation [5].

For the electron in the Coulomb field of a nucleus of charge Ze , one has

$$A_k = 0, \quad k = 1, 2, 3, \quad A_0 = -\frac{Ze}{4\pi|\mathbf{x}|} \quad [76]$$

and the time-independent equation

$$\left(-i\boldsymbol{\alpha} \cdot \nabla + \beta m - \frac{Ze^2}{4\pi|\mathbf{x}|} \right) \psi = E\psi \quad [77]$$

can be solved explicitly. This leads to a bound-state spectrum that is more accurate than its nonrelativistic counterpart. In particular, one finds that energy levels that are degenerate in the nonrelativistic theory split up into slightly different levels. The resulting fine structure of the Dirac levels can be understood as a consequence of the coupling between the spin of the electron and its orbital motion.

In spite of this better agreement with the experimental levels, the physical interpretation of the Dirac electron in a Coulomb field is enigmatic. This is not only because of the persistence of the negative-energy states of the free theory (which turn into scattering states), but also because of unphysical properties of the position operator. More general time-independent external fields (such as step potentials $A_0(\mathbf{x})$ with a step height larger than $2m$) can cause transitions between positive- and negative-energy states (Klein paradox). This phenomenon is enhanced when time dependence is allowed. In particular, any external field that is given by functions in $C_0^\infty(\mathbb{R}^4)$ leads to a scattering operator S on the one-particle space \mathcal{H} [22] that has nonzero off-diagonal parts $S_{\pm\mp}$. Hence, a positive-energy wave packet scattering at such a time- and space-localized field has a nonzero probability to show up as a negative-energy wave packet.

When one tensors the one-particle space \mathcal{H} with an internal symmetry space \mathbb{C}^k , one can also couple external Yang–Mills fields A_μ taking values in the $k \times k$ matrices via the substitution [75]. (From a geometric viewpoint, this can be rephrased as tensoring the spinor bundle with a vector bundle equipped with a connection A .) The generalization of this external gauge field coupling

to a Minkowski spacetime or Euclidean space of arbitrary dimension is straightforward. An adaptation of the resulting interacting one-particle Dirac theory in arbitrary dimension to quite general geometric settings also yields a crucial starting point for index theory.

Before turning to the latter area, we conclude this section with another striking application of the one-particle framework, namely the massless Dirac equation in two spacetime dimensions with special external fields. Specifically, the relevant Dirac operator is of the form

$$\begin{pmatrix} i \frac{d}{dx} & -iq(x) \\ ir(x) & -i \frac{d}{dx} \end{pmatrix} \quad [78]$$

where $r(x)$ and $q(x)$ are not necessarily real valued. (Note that this operator is in general not self-adjoint.) With suitable restrictions on r and q , the direct and inverse scattering theory associated with the Dirac operator [78] can be applied to various nonlinear PDEs in two spacetime dimensions to solve their Cauchy problems in considerable detail. As a crucial special case, initial conditions yielding vanishing reflection give rise to soliton solutions for the pertinent equation.

The first example in this framework was found by Zakharov and Shabat (the nonlinear Schrödinger equation); with other choices of r and q several other soliton PDEs (including the sine-Gordon and modified Korteweg–de Vries equations) were handled by Ablowitz, Kaup, Newell, and Segur, who studied a quite general class of external fields r and q .

The Dirac Operator and Index Theory

Thus far, we have considered various versions of the Dirac operator associated with the spaces \mathbb{R}^l for some $l \geq 1$. For applications in the area of index theory, however, one needs to generalize this base manifold. Indeed, one can define a Dirac operator for any l -dimensional oriented Riemannian manifold \mathcal{M} that admits a spin structure. This is a lifting of the transition functions of the tangent bundle $T\mathcal{M}$ (which may be assumed to take values in $SO(l)$) to the simply connected twofold cover $\text{Spin}(l)$ (taking $l \geq 3$).

Choosing first $l = 2N + 1$, the spin group has a faithful irreducible representation on \mathbb{C}^{2^N} . Hence, one obtains a \mathbb{C}^{2^N} -bundle over \mathcal{M} , the spinor bundle. The Levi-Civita connection on \mathcal{M} derived from the metric can now be lifted to a connection on the spinor bundle. From the covariant derivative corresponding to the spin connection and the

Clifford algebra generators $\gamma^1, \dots, \gamma^l$, one can then construct a first-order elliptic differential operator that acts on sections of the spinor bundle. (For the case $\mathcal{M} = \mathbb{R}^{2N+1}$ with its Euclidean metric, this construction yields the massless positive-chirality Dirac operator acting on wave functions with 2^N components, as considered above.)

The massless Dirac operator thus obtained is self-adjoint as an operator on the L^2 -space \mathcal{H} associated with the spinor bundle, and it has infinite-dimensional positive and negative spectral subspaces \mathcal{H}_+ and \mathcal{H}_- . (In this section the check accent on position-space quantities is omitted.) Specializing to the case of compact \mathcal{M} , a continuous map from \mathcal{M} to \mathbb{C}^* gives rise to a Fredholm operator on \mathcal{H}_+ , and more generally a continuous map from \mathcal{M} to $GL(k, \mathbb{C})$ yields a Fredholm operator on $\mathcal{H}_+ \otimes \mathbb{C}^k$.

For a smooth map, the Fredholm index of this operator can be written in terms of an integral over \mathcal{M} involving certain closed differential forms. The value of this integral does not change when exact forms are added, since \mathcal{M} has no boundary. Hence, one is dealing with de Rham cohomology classes. In this context, the class involved ("characteristic class") is determined by the Riemann curvature tensor of \mathcal{M} and the topological ("winding") characteristics of the map.

The simplest example of this state of affairs arises for $l=1$ and $\mathcal{M} = S^1$ with its obvious spin structure (periodic boundary conditions). Writing $\psi \in \mathcal{H} = L^2(S^1)$ as

$$\psi(z) = \sum_{n \in \mathbb{Z}} a_n z^n, \quad z \in S^1 \quad [79]$$

the Dirac operator H on \mathcal{H} reads

$$H = z \frac{d}{dz} \quad [80]$$

It has eigenfunctions $z^n, n \in \mathbb{Z}$. Thus, we may choose

$$(P_+ \psi)(z) = \sum_{n \geq 0} a_n z^n, \quad (P_- \psi)(z) = \sum_{n < 0} a_n z^n \quad [81]$$

As a consequence, the functions in $\mathcal{H}_+(\mathcal{H}_-)$ are L^2 -boundary values of holomorphic functions in $|z| < 1$ ($|z| > 1$). Operators of the form

$$T_\psi = P_+ M_\psi P_+ \quad [82]$$

where ψ is a continuous function on S^1 and M_ψ denotes multiplication by ψ , are called Toeplitz operators. It is not hard to see that they are Fredholm

(viewed as operators on \mathcal{H}_+), provided that ψ does not vanish on S^1 . (Recall a bounded operator B is Fredholm if it has finite-dimensional kernel K and cokernel C . Its Fredholm index is given by

$$\text{index}(B) = \dim K - \dim C \quad [83]$$

and is norm continuous and invariant under addition of a compact operator.) Assuming $\psi(S^1) \subset \mathbb{C}^*$ from now on, the curve $\psi(S^1)$ has a well-defined winding number $w(\psi)$ with respect to the origin. The equality

$$\text{index}(T_\psi) = -w(\psi) \quad [84]$$

between objects from the area of analysis on the left-hand side and from the areas of topology and geometry on the right-hand side is the simplest example of an Atiyah–Singer type index formula. When ψ is not only continuous but also smooth, the index formula can be rewritten as

$$\text{index}(T_\psi) = -\frac{1}{2\pi i} \int_{S^1} \frac{d\psi}{\psi} \quad [85]$$

yielding a characteristic class version.

It should be noted that the operator M_ψ on \mathcal{H} has a bounded inverse $M_{1/\psi}$ when $0 \notin \psi(S^1)$, hence a trivially vanishing index. Therefore, the compression [82] involving the spectral projection of the Dirac operator is needed to get a nonzero index. Observe also that the equality [84] is quite easily verified for the case $\psi(z) = z^n$, since T_ψ yields a power of the right ($n > 0$) or left ($n < 0$) shift on $P_+ \mathcal{H} \simeq l^2(\mathbb{N})$.

We proceed to the case of even-dimensional manifolds, $l=2N$. Then the fiber \mathbb{C}^{2^N} of the spinor bundle splits into a direct sum of even and odd spinors, corresponding to two distinct representations of $\text{Spin}(2N)$ on $\mathbb{C}^{2^{N-1}}$. (Here it is assumed that $N > 3$; recall the Lie algebra isomorphisms $\text{so}(4) \simeq \text{so}(3) \oplus \text{so}(3)$ and $\text{so}(6) \simeq \text{su}(4)$.) With respect to this decomposition, the Dirac operator can be written as

$$H = \begin{pmatrix} 0 & \mathcal{D}^* \\ \mathcal{D} & 0 \end{pmatrix} \quad [86]$$

where \mathcal{D} and \mathcal{D}^* are again first-order elliptic differential operators expressed in terms of Clifford algebra generators and the spin connection. Tensoring the spinor bundle with a vector bundle equipped with a connection A , one can define a Dirac operator on the tensor product which involves A and takes the form

$$H_A = \begin{pmatrix} 0 & \mathcal{D}_A^* \\ \mathcal{D}_A & 0 \end{pmatrix} \quad [87]$$

with respect to the even/odd spinor decomposition. Once more, the index of \mathcal{D}_A (viewed as a Fredholm operator between two different Hilbert spaces) can be expressed as an integral over \mathcal{M} involving characteristic classes that depend on the curvatures of the two connections.

Probably the simplest example of the constructions just sketched is given by the torus $\mathcal{M} = S^1 \times S^1$ with its flat metric. Employing the above coordinate and spin structure on S^1 , one can take

$$\mathcal{H} = L^2(S^1 \times S^1) \otimes \mathbb{C}^2, \quad \mathcal{D} = z_1 \frac{\partial}{\partial z_1} + iz_2 \frac{\partial}{\partial z_2} \quad [88]$$

Since the curvature vanishes, the index theorem for this situation implies $\text{index}(\mathcal{D}) = 0$. (Note that this is also plain from [88]: both kernel and cokernel of \mathcal{D} are spanned by the constant sections.) On the other hand, when one tensors the spinor bundle with a line bundle with connection A , the index formula reads

$$\text{index}(\mathcal{D}_A) = -\frac{1}{2\pi} \int_{S^1 \times S^1} F \quad [89]$$

where F is the curvature 2-form corresponding to A .

The Atiyah–Singer index theorem for Dirac operators has far-reaching applications. It can be used to derive other results in this area, such as the Gauss–Bonnet–Chern theorem, the Hirzebruch signature theorem, and (when \mathcal{M} is a Kähler manifold) Riemann–Roch type theorems. From this, one can obtain information on various questions, such as the existence of positive scalar curvature metrics or zeros of vector fields on \mathcal{M} . Other applications include insights on topological invariants of manifolds obtained from “simple” manifolds (such as spheres and tori) by glueing or covering operations. This hinges on the additive properties of the index that are clear from its being given by an integral over the manifold. Conversely, the integrality of Fredholm indices can be used to deduce that certain rational cohomology classes are actually integral on manifolds that admit the structure that is required for the pertinent index theorem to apply, that certain manifolds do not admit such structures, since one knows that the relevant class is not integral, etc.

More on the Dirac Field

As mentioned earlier, the free-field formalism can be easily generalized to an arbitrary spacetime dimension d . For $d > 4$, however, no renormalizable interacting quantum field models involving the Dirac field are known. For the physical case $d = 4$ the standard model involves various Dirac fields

interacting with quantized gauge fields and Klein–Gordon fields. Although its perturbation theory is renormalizable, its mathematical existence is to date wide open.

It is far beyond the scope of this article to elaborate on the analytical difficulties of relativistic quantum field theories, let alone those associated with the standard model. Even for $d = 2$ and 3, a nonperturbative construction of interacting quantum field models involving the Dirac field is an extremely difficult enterprise. Apart from some rigorous results on certain self-interacting Dirac field models, the only interacting model that is reasonably well understood from the constructive field theory viewpoint is the Yukawa model for $d = 2$ and 3. This describes the interaction between the Dirac field Ψ and a Klein–Gordon field ϕ , the interaction term being formally given by $g(\Psi^* \gamma^0 \Psi) \phi$.

On the other hand, the interaction of the quantized Dirac field with external classical fields is much more easily understood and analytically controlled. As a bonus, within this context, one can make contact with various issues of physical and mathematical relevance. We now proceed to sketch the external-field framework and some of its applications.

Let us first consider the addition of an external field term $gV(t, \mathbf{x})$ to the free Dirac operator \tilde{H} on

$$\tilde{\mathcal{H}} = L^2(\mathbb{R}^n, d\mathbf{x}) \otimes \mathbb{C}^A \otimes \mathbb{C}^k \quad [90]$$

We assume from now on that the coupling g is real and that V is a self-adjoint $k\Lambda \times k\Lambda$ matrix-valued function on spacetime \mathbb{R}^{n+1} with matrix elements that are in $C_0^\infty(\mathbb{R}^{n+1})$. Then the (interaction picture) scattering operator S exists. It is unitary and has off-diagonal Hilbert–Schmidt parts $S_{\pm\mp}$, so that a unitary Fock-space S -operator $\tilde{\Gamma}(S)$ implementing the Bogoliubov transformation generated by S exists:

$$\tilde{\Gamma}(S)\Phi(f)\tilde{\Gamma}(S)^* = \Phi(Sf), \quad \forall f \in \mathcal{H} \quad [91]$$

The arbitrary phase in $\tilde{\Gamma}(S)$ can be fixed by requiring that the vacuum expectation value of $\tilde{\Gamma}(S)$ be positive. More precisely, this number is generically nonzero and satisfies

$$|(\Omega, \tilde{\Gamma}(S)\Omega)| = \det(1 + T_S)^{-1/2} \quad [92]$$

where T_S is a positive trace class operator determined by S .

The vector $\tilde{\Gamma}(S)\Omega$ is a superposition of wave functions with an equal and arbitrary number of particles and antiparticles. More generally, the Fock-space S -operator $\tilde{\Gamma}(S)$ leaves the subspaces of $\mathcal{F}_a(\mathcal{H})$ with a fixed eigenvalue $q \in \mathbb{Z}$ of the charge operator Q invariant, and can create and

annihilate an arbitrary number of particle-antiparticle pairs.

The unitary propagator $U(T_1, T_2)$ corresponding to $V(t, \mathbf{x})$ does not have Hilbert-Schmidt off-diagonal parts (unless the spacetime dimension is sufficiently small and special external fields are chosen). Even so, the diagonal parts are Fredholm with vanishing index, and the off-diagonal parts are compact. Omitting the ill-defined determinantal factor, these properties imply that one obtains a renormalized quadratic form $\tilde{\Gamma}_{\text{rcn}}(U(T_1, T_2))$ satisfying the implementing relation

$$\begin{aligned} \tilde{\Gamma}_{\text{rcn}}(U(T_1, T_2))\Phi(f) \\ = \Phi(U(T_1, T_2)f)\tilde{\Gamma}_{\text{rcn}}(U(T_1, T_2)), \quad \forall f \in \mathcal{H} \end{aligned} \quad [93]$$

in the quadratic form sense.

The above unitary operators on \mathcal{H} yield Fredholm diagonal parts whose indices vanish. (They are norm continuous in g and reduce to the identity for $g=0$.) This is why their Fock-space implementers leave the charge sectors invariant. Indeed, for a unitary operator U on \mathcal{H} with compact off-diagonal parts the implementer maps the charge- q sector to the charge- $(q + q(U))$ sector, where

$$q(U) = \text{index}(U_{--}) \quad [94]$$

Specializing to the case

$$n = 2N - 1, \quad \Lambda = 2\lambda, \quad \lambda = 2^{N-1} \quad [95]$$

a unitary $(k\Lambda \times k\Lambda)$ -matrix multiplier \check{U} on $\check{\mathcal{H}}$ does not have compact off-diagonal parts in general. But when it is of the form

$$\check{U} = \begin{pmatrix} \mathbf{1}_\lambda \otimes u_+(\mathbf{x}) & 0 \\ 0 & \mathbf{1}_\lambda \otimes u_-(\mathbf{x}) \end{pmatrix} \quad [96]$$

with respect to the chiral decomposition (the generalization of the γ^5 -decomposition [72] to even spacetime dimension), then it suffices for compactness of the off-diagonal parts that the matrices $u_\pm(\mathbf{x}) \in U(k)$ are continuous and converge to $\mathbf{1}_k$ for $|\mathbf{x}| \rightarrow \infty$.

Viewing \mathbb{R}^{2N-1} as arising from S^{2N-1} via stereographic projection, the latter unitaries can be viewed as continuous maps from S^{2N-1} to $U(k)$, reducing to $\mathbf{1}_k$ at the north pole. As such, they yield elements of the homotopy group $\pi_{2N-1}(U(k))$. By virtue of Bott's periodicity theorem, the latter group equals \mathbb{Z} for $k \geq N$. Thus, the maps u_\pm have a well-defined "winding number" $w(u_\pm) \in \mathbb{Z}$ for $k \geq N$. From the index formula

$$\text{index}(U_{--}) = w(u_+) - w(u_-) \quad [97]$$

and [94] one now deduces that one can obtain implementers $\tilde{\Gamma}_{\text{rcn}}(U)$ effecting a nonzero charge

change from unitary maps with nonzero winding number.

In particular, choosing $k = \lambda = 2^{N-1} \geq N$, there exist quite special "kink maps"

$$u_{\epsilon,a}(\mathbf{x}) \in U(\lambda), \quad \epsilon > 0, \quad a \in \mathbb{R}^{2N-1} \quad [98]$$

with winding number 1 and such that the quadratic form implementers of the unitary multiplication operators

$$\begin{aligned} \check{U}_{+,\epsilon,a} &= - \begin{pmatrix} \mathbf{1}_\lambda \otimes u_{\epsilon,a}(\mathbf{x}) & 0 \\ 0 & \mathbf{1}_\lambda \otimes \mathbf{1}_\lambda \end{pmatrix} \\ \check{U}_{-,\epsilon,a} &= - \begin{pmatrix} \mathbf{1}_\lambda \otimes \mathbf{1}_\lambda & 0 \\ 0 & \mathbf{1}_\lambda \otimes u_{\epsilon,a}(-\mathbf{x}) \end{pmatrix} \end{aligned} \quad [99]$$

converge to (a linear combination of the chiral components of) the free Dirac field $\Psi(0, a)$ as the kink size parameter ϵ goes to 0.

For the special case $N=1$, one can take

$$u_{\epsilon,a}(\mathbf{x}) = \frac{x - a - i\epsilon}{x - a + i\epsilon} \quad [100]$$

and the off-diagonal parts of $U_{\pm,\epsilon,a}$ are actually Hilbert-Schmidt. Thus, the implementers can be chosen to be unitary operators. But to get convergence to the Dirac field components $\Psi(0, a)_\pm$ as $\epsilon \rightarrow 0$, the unitary implementers $\tilde{\Gamma}(U_{\pm,\epsilon,a})$ should be renormalized by a multiplicative factor.

For the $N=1$ case, the unitary multipliers [96] give rise to loop groups. Indeed, requiring

$$\lim_{x \rightarrow \pm\infty} u_\delta(x) = \mathbf{1}_k, \quad \delta = +, - \quad [101]$$

we are dealing with continuous maps $S^1 \rightarrow U(k)$. From the viewpoint of the Dirac theory, these groups are local gauge groups. The convergence to the Dirac field just sketched can be used to great advantage to clarify the structure of the corresponding Fock-space gauge groups. Their Lie algebras yield representations of Kac-Moody algebras, a topic which is considered shortly.

Before doing so, it should be pointed out that under some mild smoothness assumptions all of the above unitary matrix multipliers can also be viewed as S -operators associated with very special external fields. Indeed, the gauge-transformed Dirac operator

$$\check{H}_U = \check{U}^* \check{H} \check{U} \quad [102]$$

is of the form

$$\check{H}_U = \check{H} + V(\mathbf{x}) \quad [103]$$

where $V(x)$ is a self-adjoint $k\Lambda \times k\Lambda$ matrix on \mathbb{R}^{2N-1} (a “pure gauge” field). If one now defines a time-dependent external field by

$$V(t, x) = \begin{cases} V(x), & t \geq 0 \\ 0, & t < 0 \end{cases} \quad [104]$$

then \check{U} equals the S -operator for $V(t, x)$. (Equivalently, \check{U} is the $t \rightarrow \infty$ wave operator for the time-independent external field $V(x)$.)

To conclude this section we sketch some applications of the second-quantized Dirac formalism for the special case $N=1$, $m=0$, and positive chirality. Even though we could stick to the massless positive-chirality Dirac operator $-id/dx$ on the line, it is simpler and more natural to start from its counterpart on the circle already considered in the last section, cf. [80]. (Under the Cayley transform, the positive- and negative-energy subspaces of $-id/dx$ on $L^2(\mathbb{R})$ correspond to those of zd/dz on $L^2(S^1)$, given by [81].) Letting $z=e^{i\theta}$, we then obtain

$$\begin{aligned} \check{H} &= -id/d\theta, \quad \check{\mathcal{H}} = L^2([0, 2\pi], d\theta) \\ \mathcal{H} &= l^2(\mathbb{Z}), \quad \mathcal{H}_+ = l^2(\mathbb{N}), \quad \mathcal{H}_- = l^2(\mathbb{Z}_-) \end{aligned} \quad [105]$$

and a corresponding Dirac field

$$\begin{aligned} \Psi(t, \theta) &= (2\pi)^{-1/2} \left(\sum_{n=0}^{\infty} a_n e^{-int+i\theta} + \sum_{n=1}^{\infty} b_{-n}^* e^{int-i\theta} \right) \\ (t, \theta) &\in \mathbb{R} \times [0, 2\pi] \end{aligned} \quad [106]$$

where

$$a_l = c(e_l), \quad l \geq 0, \quad b_l = c(e_l), \quad l < 0 \quad [107]$$

and $\{e_l\}_{l \in \mathbb{Z}}$ is the canonical basis of $l^2(\mathbb{Z})$.

Consider now the group $GL(\mathcal{H})$ of bounded operators on \mathcal{H} with bounded inverses. The transformation

$$\begin{aligned} \Phi^*(f) &\mapsto \Phi^*(Gf), \quad \Phi(f) \mapsto \Phi(G^{-1*}f) \\ f &\in \mathcal{H}, \quad G \in GL(\mathcal{H}) \end{aligned} \quad [108]$$

leaves the CAR [48] invariant. Provided that G belongs to the subgroup

$$\begin{aligned} G_2(\mathcal{H}) &= \{G \in GL(\mathcal{H}) \mid G_{\pm\mp} \text{ Hilbert-Schmidt} \} \end{aligned} \quad [109]$$

there exists an implementer $\tilde{\Gamma}(G)$ on $\mathcal{F}_a(\mathcal{H})$:

$$\begin{aligned} \tilde{\Gamma}(G)\Phi^*(f) &= \Phi^*(Gf)\tilde{\Gamma}(G), \\ \tilde{\Gamma}(G)\Phi(f) &= \Phi(G^{-1*}f)\tilde{\Gamma}(G), \quad \forall f \in \mathcal{H} \end{aligned} \quad [110]$$

In particular, the multiplication operator

$$\exp(h(x)), \quad h(x) = \sum_{k=1}^{\infty} x_k z^{-k}, \quad z = e^{i\theta} \quad [111]$$

belongs to $G_2(\mathcal{H})$ provided the sequence x_k vanishes sufficiently fast as $k \rightarrow \infty$. Thus, one obtains an implementer $\tilde{\Gamma}(e^{h(x)})$, the so-called KP evolution operator. This designation is justified by the vacuum expectation value

$$\tau(x) = (\Omega, \tilde{\Gamma}(e^{h(x)})\tilde{\Gamma}(G)\Omega), \quad G \in G_2(\mathcal{H}) \quad [112]$$

being a tau-function solving the hierarchy of KP evolution equations in Hirota bilinear form, as first shown by Sato and his Kyoto school. For example, the KP equation itself,

$$u_{yy} = \partial_x \left(\frac{4}{3} u_t - 2uu_x - \frac{1}{3} u_{xxx} \right) \quad [113]$$

has the bilinear form

$$\begin{aligned} \left(\frac{\partial^4}{\partial y_1^4} - 4 \frac{\partial}{\partial y_1} \frac{\partial}{\partial y_3} + 3 \frac{\partial^2}{\partial y_2^2} \right) \tau(x+y) \tau(x-y) \Big|_{y=0} \\ = 0 \end{aligned} \quad [114]$$

the relation being given by

$$x_1 = x, \quad x_2 = y, \quad x_3 = t, \quad u = 2\partial_1^2 \ln \tau \quad [115]$$

The class of solutions to [113] thus obtained includes not only the rational and soliton solutions (which correspond to choosing \tilde{G} as multiplication by a rational function of $z=e^{i\theta}$ that does not vanish on S^1), but also the finite-gap solutions associated with compact Riemann surfaces. Moreover, for suitable subgroups of $G_2(\mathcal{H})$, one obtains tau-functions for related soliton hierarchies, including the Korteweg-de Vries, Boussinesq and Hirota-Satsuma hierarchies. Even though the class of solutions associated with $G_2(\mathcal{H})$ via the Dirac formalism is large, it should be noted that from the perspective of the Cauchy problem for the pertinent evolution equations the solutions are nongeneric, inasmuch as the initial data are real-analytic functions.

Finally, we consider Lie algebra representations related to the above special starting point [105] for the second-quantized Dirac framework. Assume that $\exp(tA)$ is a one-parameter group of bounded operators on \mathcal{H} with generator A in the Lie algebra of $G_2(\mathcal{H})$,

$$\begin{aligned} g_2(\mathcal{H}) &= \{A \text{ bounded} \mid A_{\pm\mp} \text{ Hilbert-Schmidt} \} \end{aligned} \quad [116]$$

Then one can take

$$\tilde{\Gamma}(\exp(tA)) = \exp(td\tilde{\Gamma}(A)) \quad [117]$$

where $d\tilde{\Gamma}(A)$ is the Fock-space operator uniquely determined up to an additive constant by its commutation relation

$$[d\tilde{\Gamma}(A), \Phi^*(f)] = \Phi^*(Af), \quad \forall f \in \mathcal{H} \quad [118]$$

with the smeared Dirac field $\Phi^*(f)$. Fixing the constant by requiring

$$(\Omega, d\tilde{\Gamma}(A)\Omega) = 0 \quad [119]$$

the map $A \mapsto d\tilde{\Gamma}(A)$ satisfies the Lie algebra relations

$$[d\tilde{\Gamma}(A), d\tilde{\Gamma}(B)] = d\tilde{\Gamma}([A, B]) + C(A, B)1 \quad [120]$$

so that the term

$$C(A, B) = \text{tr}(A_{-+}B_{+-} - B_{-+}A_{+-}) \quad [121]$$

encodes a central extension of the Lie algebra $\mathfrak{g}_2(\mathcal{H})$ [116].

The developments sketched in the previous paragraph are in fact independent of the specific form of the Hilbert space \mathcal{H} and its $\mathcal{H}_+/\mathcal{H}_-$ decomposition. But the special feature of the choice [105] and its $S^1 \rightarrow \mathbb{R}$ analog is that the smeared Dirac current

$$\int_0^{2\pi} d\theta \psi(\theta) : \Psi^*(0, \theta) \Psi(0, \theta) :, \quad \psi \in C^\infty(S^1) \quad [122]$$

(where the double dots denote normal ordering – the replacement of terms involving $b_k b_l^*$ by $-b_l^* b_k$) is of the form $d\tilde{\Gamma}(A_\psi)$ with $A_\psi \in \mathfrak{g}_2(\mathcal{H})$ determined by ψ . (For spacetime dimension $d > 2$, this is no longer true, as the Hilbert–Schmidt condition is violated.) Moreover, [120] reduces to

$$[d\tilde{\Gamma}(A_\psi), d\tilde{\Gamma}(A_\phi)] = C(A_\psi, A_\phi)1 \quad [123]$$

with the central extension explicitly given by

$$C(A_\psi, A_\phi) = \frac{i}{2\pi} \int_0^{2\pi} d\theta \psi'(\theta) \phi(\theta) \quad [124]$$

We have just sketched the details of the (simplest version of the) Dirac current algebra: the term [124] is commonly known as the Schwinger term, so that the central extension featuring in [120]–[121] may be viewed as a generalization. The above setup can also be slightly generalized so as to obtain representations of the Virasoro algebra, which is a central extension of the Lie algebra of polynomial vector fields on S^1 . The general framework has a quite similar version for the neutral Dirac field (Majorana field), described in terms of the self-dual CAR algebra. In the neutral setting, one can construct the Neveu–Schwarz and Ramond representations of the Virasoro algebra, which are crucial in string theory.

Tensoring $\tilde{\mathcal{H}}$ with an internal symmetry space \mathbb{C}^k and starting from the Lie algebra of rational maps $S^1 \rightarrow \mathfrak{sl}(k, \mathbb{C})$, $z \mapsto M(z)$, with poles occurring solely

at $z=0$ and $z=\infty$ (regarded as multiplication operators on $L^2(S^1)^k$), the Fock-space counterparts obtained via the $d\tilde{\Gamma}$ -operation yield representations of the Kac–Moody Lie algebra $A_{k-1}^{(1)}$. Specifically, on the charge-0 sector of $\mathcal{F}_a(\mathcal{H})$, one obtains the so-called basic representation, whereas the charge- q sectors with $q=1, \dots, k-1$, yield the fundamental representations. Using the neutral version of Dirac’s second quantization, one can also obtain the basic and a fundamental representation of the Kac–Moody algebras $B_l^{(1)}$ (for $k=2l+1$) and $D_l^{(1)}$ (for $k=2l$).

See also: Bosons and Fermions in External Fields; Clifford Algebras and Their Representations; Current Algebra; Dirac Fields in Gravitation and Nonabelian Gauge Theory; Gerbes in Quantum Field Theory; Holonomic Quantum Fields; Index Theorems; Quantum Field Theory in Curved Spacetime; Quantum Chromodynamics; Random Walks in Random Environments; Relativistic Wave Equations Including Higher Spin Fields; Solitons and Kac–Moody Lie Algebras; Spinors and Spin Coefficients; Symmetry Classes in Random Matrix Theory.

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Dispersion Relations

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Introduction

Dispersion relations constitute a basic chapter of mathematical physics which covers various types of classical and quantum scattering phenomena and illustrates in a typical way the importance of general principles in theoretical physics, among which causality plays a major role. Each such phenomenon is described in terms of a scattering amplitude $F(\omega)$, which is a complex-valued function of a frequency variable ω ; in quantum physics, this variable becomes an energy variable called E (or s in particle physics), as it follows from the fundamental de Broglie relation $E = \hbar\omega$. The real and imaginary parts of $F(\omega)$, which are called respectively the dispersive part $D(\omega)$ and the absorptive part $A(\omega)$ of F , have well-defined physical interpretations for all these phenomena; they represent quantities which are essentially accessible to measurements. The term dispersion relations refers to linear integral equations which relate the functions $D(\omega)$ and $A(\omega)$; such integral equations are always closely related to the Cauchy integral representation of a subjacent holomorphic function $\hat{F}(\omega^{(c)})$ of the complexified frequency (or energy) variable $\omega^{(c)}$. $\hat{F}(\omega^{(c)})$ is called the holomorphic scattering function or in short the scattering function, and the scattering amplitude appears as the boundary value of the latter, taken at positive real values of ω from the upper half-plane of $\omega^{(c)}$, namely

$$F(\omega) = \lim_{\varepsilon \rightarrow 0} \hat{F}(\omega + i\varepsilon), \quad \varepsilon > 0$$

Historically, the first relations of that type to be obtained were the Kramers–Krönig relations (1926), which concern the propagation of light in a dielectric medium. In this basic example, $F(\omega)$ represents the complex refractive index of the medium $n'(\omega) = n(\omega) + i\kappa(\omega)$ for a monochromatic wave with frequency ω . The dispersive part $D(\omega)$ is the real refractive index $n(\omega)$, which is the inverse ratio of the phase velocity of the wave in the medium to its velocity c in the vacuum: the fact that it depends on the frequency ω corresponds precisely to the phenomenon of dispersion of light in a dielectric medium. A slab of the latter thus appears as a prototype of a macroscopic scatterer. The absorptive part $A(\omega)$ is the rate of exponential

damping $\kappa(\omega)$ of the wave, caused by the absorption of energy in the medium.

It has appeared much later that for many scattering phenomena, dispersion relations can be derived from an appropriate set of general physical principles. This means that inside a certain axiomatic framework these relations are model independent with respect to the detailed structure of the scatterer or to the detailed type of particle interaction in the quantum case.

In a very short and oversimplifying way, the following logical scheme holds. At first, one can say that any mathematical formulation of a physical principle of causality results in support-type properties with respect to a time variable t of an appropriate “causal structural function” $R(t)$ of the physical system considered: typically, such a causal function should vanish for negative values of t . It follows that its Fourier transform \hat{R} admits an analytic continuation $\hat{R}^{(c)}$ in the upper half-plane of the corresponding conjugate variable, interpreted as a frequency (or an energy in the quantum case): here is the general reason for the occurrence of complex frequencies and of holomorphic functions of such variables. In fact, the relevant holomorphic scattering function $\hat{F}(\omega^{(c)})$ always appears as generated by $\hat{R}^{(c)}$ via some (more or less sophisticated) procedure: in the simplest case, \hat{F} coincides with $\hat{R}^{(c)}$ itself, but this is not so in general. Finally, the derivation of suitable analyticity and boundedness properties of $\hat{F}(\omega^{(c)})$ in a domain whose typical form is the upper half-plane, allows one to apply a Cauchy-type integral representation to this function; the dispersion relations directly follow from the latter.

The first part of this article aims to describe the most typical dispersion relations and their link with the Cauchy integral. It then presents two basic illustrations of these relations, which are: (1) in classical physics, the Kramers–Krönig relations mentioned above, and (2) in quantum physics, the dispersion relations for the forward scattering of equal-mass particles. The aim of the subsequent parts is to give as complete as possible accounts of the derivation of the relevant analyticity domains inside appropriate axiomatic frameworks which, respectively, contain the previous two examples. The simplest axiomatic framework is the one which governs all the phenomena of linear response: in the latter, the proof of analyticity and dispersion relations most easily follows the logical line sketched above. It will be presented together with its application to the derivation of

the Kramers–Krönig relations. The rest of the article is devoted to the derivation of the so-called crossing analyticity domains which are the relevant background of dispersion relations for the two-particle scattering (or collision) amplitudes in particle physics. This derivation relies on the general axiomatic framework of relativistic quantum field theory (QFT) (see Axiomatic Quantum Field Theory) and more specifically on the “analytic program in complex momentum space” of the latter. This framework, whose rigorous mathematical form has been settled around 1960, represents the safest conceptual approach for describing the particle collision processes in a range of energies which covers by far all those that can be produced and will be produced in the accelerators for several decades. A simple account of the field-theoretical axiomatic framework and of the logical line of the derivation of dispersion relations will be presented here for the simplest kinematical situations. A broader presentation of the analytic program including an extended class of analyticity properties for the general structure functions and (two-particle and multiparticle) collision amplitudes in QFT can also be found in this encyclopedia (see Scattering in Relativistic Quantum Field Theory: The Analytic Program). For brevity, we shall not treat here the derivation of dispersion relations in the framework of nonrelativistic potential theory. Concerning the latter, the interested reader can refer to the book by Nussenzweig (1972). A collection of old basic papers on field-theoretical dispersion relations can be found in the review book edited by Klein (1961). For a recent and well-documented review of the multiplicity of versions and applications of dispersion relations and their experimental checking, the reader can consult the article by Vernov (1996).

Typical Dispersion Relations

The possibility of defining the scattering function $\hat{F}(\omega^{(c)})$ in the full upper half-plane and of exploiting the corresponding boundary value F of \hat{F} on the negative part as well as on the positive part of the real axis will depend on the framework of considered phenomena. For the moment, we do not consider the more general situations which also occur in particle physics and will be described later (“crossing domains” and “quasi-dispersion-relations”).

In the simplest cases, the real and imaginary parts D and A of F are extended to negative values of the variable ω via additional symmetry relations resulting from appropriate “reality conditions.” As a typical and basic example, there occurs the

symmetry relation $\overline{\hat{F}(\omega^{(c)})} = \hat{F}(-\overline{\omega^{(c)}})$, (with $\omega^{(c)}$ and $-\overline{\omega^{(c)}}$ in the upper half-plane) and correspondingly $D(\omega) = D(-\omega)$, $A(\omega) = -A(-\omega)$ on the reals; we shall call (S) this symmetry relation.

The simplest case of dispersion relations is then obtained when D and A are linked by the reciprocal Hilbert transformations:

$$D(\omega) = \frac{1}{\pi} P \int_{-\infty}^{+\infty} A(\omega') \frac{1}{\omega' - \omega} d\omega' \quad [1a]$$

$$A(\omega) = -\frac{1}{\pi} P \int_{-\infty}^{+\infty} D(\omega') \frac{1}{\omega' - \omega} d\omega' \quad [1b]$$

where P denotes Cauchy’s principal value, defined for any differentiable function $\varphi(x)$ (sufficiently regular at infinity) by

$$\begin{aligned} P \int_{-\infty}^{+\infty} \frac{\varphi(x)}{x} dx \\ = \lim_{\varepsilon \rightarrow 0} \left[\int_{-\infty}^{-\varepsilon} \varphi(x) \frac{dx}{x} + \int_{\varepsilon}^{+\infty} \varphi(x) \frac{dx}{x} \right] \end{aligned} \quad [2]$$

As a matter of fact, the pair of equations [1a], [1b] is equivalent to the following relation for $F \doteq D + iA$:

$$F(\omega) = \frac{1}{2i\pi} \int_{-\infty}^{+\infty} F(\omega') \lim_{\varepsilon \rightarrow 0} \frac{1}{\omega' - \omega - i\varepsilon} d\omega' \quad [3]$$

The latter is obtained as a limiting case of the Cauchy formula

$$\hat{F}(\omega^{(c)}) = \frac{1}{2i\pi} \int_{-\infty}^{+\infty} \frac{F(\omega')}{\omega' - \omega^{(c)}} d\omega' \quad [4]$$

expressing the fact that \hat{F} is holomorphic and sufficiently decreasing at infinity in the upper half-plane \mathcal{I}_+ of the complex variable $\omega^{(c)}$ and that $F(\omega)$ is the boundary value of $\hat{F}(\omega^{(c)})$ on all the reals.

Finally, one checks that in view of the symmetry relation (S), the Hilbert integral relations between D and A given above reduce to the following dispersion relations:

$$D(\omega) = \frac{2}{\pi} P \int_0^{+\infty} A(\omega') \frac{\omega'}{\omega'^2 - \omega^2} d\omega' \quad [5a]$$

$$A(\omega) = -\frac{2\omega}{\pi} P \int_0^{+\infty} D(\omega') \frac{1}{\omega'^2 - \omega^2} d\omega' \quad [5b]$$

Two Basic Examples

1. *The Kramers–Krönig relation in classical optics*
It will be shown in the next part that the complex refractive index $n'(\omega) = n(\omega) + i\kappa(\omega)$ of a dielectric medium is the boundary value of a holomorphic

function $\hat{n}'(\omega^{(c)})$ in \mathcal{I}_+ satisfying the symmetry relation (S), and such that the integral $\int_{-\infty}^{\infty} |\hat{n}'(\omega + i\eta) - 1|^2 d\omega$ is uniformly bounded for all $\eta > 0$.

It follows that all the previous relations are satisfied by the function $\hat{F}(\omega^{(c)}) = \hat{n}'(\omega^{(c)}) - 1$. In particular, the real refractive index $n(\omega)$ and the "extinction coefficient" $\beta(\omega) \doteq 2\omega\kappa(\omega)/c$ (c being the velocity of light in the vacuum) are linked by the following Kramers–Krönig dispersion relation (corresponding to eqn [5a]):

$$n(\omega) - 1 = \frac{c}{2\pi} P \int \frac{\beta(\omega')}{\omega'^2 - \omega^2} d\omega' \quad [6]$$

2. Dispersion relation for the forward two-particle scattering amplitude in relativistic quantum physics
One considers the following collision phenomenon in particle physics. A particle Π_2 with mass m , called the target and sitting at rest in the laboratory, is collided by an identical particle Π_1 with relativistic energy ω larger than m ($=mc^2$; in high-energy physics, one usually chooses units such that $c=1$). After the collision, the particle Π_1 is scattered in all possible directions, θ , of space, according to a certain quantum scattering amplitude $T_\theta(\omega)$, whose modulus is essentially the rate of probability for detecting Π_1 in the direction θ . The forward scattering amplitude $T_0(\omega)$ corresponds to the detection of Π_2 in the forward longitudinal direction with respect to its incidence direction towards the target. Let us also assume that the particles carry no charge of any kind, so that each particle coincides with its "antiparticle." In that case, $T_0(\omega)$ is shown to be the boundary value of a scattering function $\hat{T}_0(\omega^{(c)})$ enjoying the following properties:

1. it is a holomorphic function in \mathcal{I}_+ satisfying the symmetry relation (S);
2. its behavior at infinity in \mathcal{I}_+ is such that the integral

$$\int_{-\infty}^{\infty} \left| \frac{\hat{T}_0(\omega + i\eta)}{(\omega + i\eta)^2} \right|^2 d\omega$$

is uniformly bounded for all $\eta > 0$; and

3. under more specific assumptions on the mass spectrum of the subjacent theory, the "absorptive part" $A(\omega) \doteq \text{Im } T_0(\omega)$ vanishes for $|\omega| < m$.

Then by applying eqn [5a] to the function $D(\omega) \doteq \text{Re}[(T_0(\omega) - T_0(0))/\omega^2]$ (regular at $\omega=0$), one obtains the following dispersion relation:

$$\begin{aligned} \text{Re } T_0(\omega) \\ = T_0(0) + \frac{2\omega^2}{\pi} P \int_m^{+\infty} A(\omega') \frac{1}{\omega'(\omega'^2 - \omega^2)} d\omega' \quad [7] \end{aligned}$$

Remark In view of (3), the scattering function $\hat{T}_0(\omega^{(c)})$ admits an analytic continuation as an even function of $\omega^{(c)}$ (still called \hat{T}_0) in the cut-plane $C_m^{(\text{cut})} \doteq C \setminus \{\omega \in \mathbb{R}; |\omega| \geq m\}$. In fact, in view of (S) and (3), the boundary value T_0 of \hat{T}_0 satisfies the relation $T_0(\omega) = T_0(-\omega)$ in the real interval $\delta_m \doteq \{\omega \in \mathbb{R}; -m < \omega < m\}$. Let us then introduce the function $\hat{T}_0^-(\omega^{(c)}) \doteq \hat{T}_0(-\omega^{(c)})$ as a holomorphic function of $\omega^{(c)}$ in \mathcal{I}_- : one sees that the boundary values of \hat{T}_0 and \hat{T}_0^- from the respective domains \mathcal{I}_+ and \mathcal{I}_- coincide on δ_m and therefore admit a common analytic continuation throughout this real interval (in view of "Painlevé's lemma" or "one-dimensional edge-of-the-wedge theorem"). One also notes that in view of (S) the extended function \hat{T}_0 satisfies the "reality condition" $\hat{T}_0(\omega^{(c)}) = \hat{T}_0(\overline{\omega^{(c)}})$ in $C_m^{(\text{cut})}$. The fact that \hat{T}_0 is well defined as an even holomorphic function in the cut-plane $C_m^{(\text{cut})}$ has been established in the general framework of QFT, as explained in the last part of this article.

Phenomena of Linear Response: Causality and Dispersion Relations in the Classical Domain

The subsequent axiomatic framework and results (due to J S Toll (1952, 1956)) concern any physical system which exhibits the following type of phenomena: whenever it receives some excitation signal, called the input and represented by a real-valued function of time $f_{\text{in}}(t)$ with compact support, the system emits a response signal, called the output and represented by a corresponding real-valued function $f_{\text{out}}(t)$, in such a way that the following postulates are satisfied:

- (P1) *Linearity.* To every linear combination of inputs $a_1 f_{\text{in},1} + a_2 f_{\text{in},2}$, there corresponds the output $a_1 f_{\text{out},1} + a_2 f_{\text{out},2}$.
- (P2) *Reproductibility or time-translation invariance.* Let τ be a time-translation parameter taking arbitrary real values; to every "time-translated input" $f_{\text{in}}^{(\tau)}(t) \doteq f_{\text{in}}(t - \tau)$, there corresponds the output $f_{\text{out}}^{(\tau)}(t) \doteq f_{\text{out}}(t - \tau)$.
- (P3) *Causality.* The effect cannot precede the cause, namely if t_{in} and t_{out} denote respectively the lower bounds of the supports of $f_{\text{in}}(t)$ and $f_{\text{out}}(t)$, then there always holds the inequality $t_{\text{in}} \leq t_{\text{out}}$.
- (P4) *Continuity of the response.* There exists some continuity inequality which expresses the fact that a certain norm of the output is majorized by a corresponding norm of the input. The case of an L_2 -norm inequality of the

form $|f_{\text{out}}| \leq |f_{\text{in}}|$ is particularly significant: when the norm $|f| \doteq [\int |f(t)|^2 dt]^{1/2}$ is interpretable as an energy (for the output as well as for the input), it acquires the meaning of a “dissipation” property of the system.

The postulate of linear dependence (P1) of f_{out} with respect to f_{in} is obviously satisfied if the response is described by any general kernel $K(t, t')$ such that the following formula makes sense:

$$f_{\text{out}}(t) = \int_{-\infty}^{+\infty} K(t, t') f_{\text{in}}(t') dt' \quad [8]$$

Conversely, the existence of a distribution kernel K can be established rigorously under the continuity assumption postulated in (P4) by using the Schwartz nuclear theorem. In full generality (see our comment in the next paragraph), the kernel $K(t, t')$ appears to be a tempered distribution in the pair of variables (t, t') and the previous integral formula holds in the sense of distributions, which means that both sides of eqn [8] must be considered as tempered distributions (in t) acting on any smooth test-function $g(t)$ in the Schwartz space \mathcal{S} . (Note, for instance, that the trivial linear application $f_{\text{out}} = f_{\text{in}}$ is represented by the kernel $K(t, t') = \delta(t - t')$).

From the reproductibility postulate (P2), it follows that the distribution K can be identified with a distribution of the single variable $\tau = t - t'$, namely $K(t, t') \doteq R(t - t')$. Moreover, the real-valuedness condition imposed to the pairs $(f_{\text{in}}, f_{\text{out}})$ entails that R is real. Finally, the causality postulate (P3) implies that the support of the distribution R is contained in the positive real axis, so that one can write, in the sense of distributions,

$$f_{\text{out}}(t) = \int_{-\infty}^t R(t - t') f_{\text{in}}(t') dt' \quad [9]$$

The convolution kernel $R(t - t')$ is typically what one calls in physics a “retarded kernel.”

If we now introduce the frequency variable ω , which is the conjugate of the time variable t , by the Fourier transformation

$$\tilde{f}(\omega) = \int_{-\infty}^{+\infty} f(t) e^{i\omega t} dt$$

we see that the convolution equation [9] is equivalent to the following one:

$$\tilde{f}_{\text{out}}(\omega) = \tilde{R}(\omega) \tilde{f}_{\text{in}}(\omega) \quad [10]$$

In the latter, the Fourier transform $\tilde{R}(\omega)$ of R is a tempered distribution, which is the boundary value from the upper half-plane \mathcal{I}_+ of a holomorphic

function $\tilde{R}^{(c)}(\omega^{(c)})$, called the Fourier–Laplace transform of R . $\tilde{R}^{(c)}$ is defined for all $\omega^{(c)} = \omega + i\eta$, with $\eta > 0$, by the following formula in which the exponential is a good test-function for the distribution R (since exponentially decreasing for $t \rightarrow +\infty$):

$$\tilde{R}^{(c)}(\omega^{(c)}) = \int_0^{+\infty} R(t) e^{i\omega^{(c)} t} dt \quad [11]$$

More precisely, the tempered-distribution character of R is strictly equivalent to the fact that $\tilde{R}^{(c)}$ is of moderate growth both at infinity and near the reals in \mathcal{I}_+ , namely that it satisfies a majorization of the following form for some real positive numbers p and q :

$$|\tilde{R}^{(c)}(\omega + i\eta)| \leq C \frac{(1 + |\omega|^2 + \eta^2)^q}{\eta^p} \quad [12]$$

We thus conclude from eqn [10] that each phenomenon of linear response is represented very simply in the frequency variable by the multiplicative operator $\tilde{R}(\omega)$, whose analytic continuation $\tilde{R}^{(c)}(\omega^{(c)})$ is called the (causal) response function.

A Typical Illustration: The Damped Harmonic Oscillator

We consider the motion $x = x(t)$ of a damped harmonic oscillator of mass m submitted to an external force $F(t)$. The force is the input ($f_{\text{in}} = F$) and the resulting motion is the output, namely $f_{\text{out}}(t) = x(t)$. All the previous general postulates (P1)–(P4) are then satisfied, but this particular model is, of course, governed by its dynamical equation

$$x''(t) + 2\gamma x'(t) + \omega_0^2 x(t) = \frac{F(t)}{m} \quad [13]$$

where ω_0 is the eigenfrequency of the oscillator and γ is the damping constant ($\gamma > 0$). The relevant solution of this second-order differential equation with constant coefficients is readily obtained in terms of the Fourier transforms $\tilde{x}(\omega)$ of $x(t)$ and $\tilde{F}(\omega)$ of $F(t)$. One can in fact replace eqn [13] by the equivalent equation

$$(-\omega^2 - 2i\gamma\omega + \omega_0^2) \tilde{x}(\omega) = \frac{\tilde{F}(\omega)}{m} \quad [14]$$

whose solution is of the form [10], namely $\tilde{x}(\omega) = \tilde{R}(\omega) \tilde{F}(\omega)$, with

$$\begin{aligned} \tilde{R}(\omega) &= -\frac{\tilde{F}(\omega)}{m(\omega^2 + 2i\gamma\omega - \omega_0^2)} \\ &= -\frac{\tilde{F}(\omega)}{m(\omega - \omega_1)(\omega - \omega_2)} \end{aligned} \quad [15a]$$

$$\omega_{1,2} = \pm(\omega_0^2 - \gamma^2)^{1/2} - i\gamma \quad [15b]$$

It is clear that the rational function defined by eqns [15] admits an analytic continuation in the full complex plane of $\omega^{(c)}$ minus the pair of simple poles (ω_1, ω_2) which lie in the lower half-plane. In particular, it is holomorphic (and decreasing at infinity) in \mathcal{I}_+ , as expected from the previous general result. Moreover, this example suggests that for any particular phenomenon of linear response, the details of the dynamics are encoded in the singularities of the holomorphic scattering function $\tilde{R}^{(c)}(\omega^{(c)})$, which all lie in the lower half-plane. The validity of a dispersion relation only expresses the analyticity (and decrease at infinity) of that function in the upper half-plane, which is model independent.

Remark The same mathematical analysis applies to any electric oscillatory circuit, in which the capacitance, inductance, and resistance are involved in place of the parameters m , ω_0 and γ : f_{in} and f_{out} correspond respectively to an external electric potential and to the current induced in the circuit; the response function is the admittance of the circuit.

Application to the Kramers–Krönig Relation

The background of the Kramers–Krönig relation [6], namely the analyticity and boundedness properties of the complex refractive index $\hat{n}'(\omega^{(c)})$ in \mathcal{I}_+ , is provided by the previous axiomatic framework. However, it is not the quantity $\hat{n}'(\omega^{(c)})$ itself but appropriate functions of the latter which play the role of causal response functions; two phenomena can in fact be exhibited, which both contribute to proving the relevant properties of $\hat{n}'(\omega^{(c)})$.

1. *Propagation of light in a dielectric slab with thickness δ .* One considers the wave front $f_{\text{in}}(t)$ of an incoming wave normally incident upon the slab, with Fourier decomposition

$$f_{\text{in}}(t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \tilde{f}(\omega) e^{-i\omega t} d\omega \quad [16]$$

After having traveled through the medium, it gives rise to an outgoing wave $f_{\text{out}}(t)$ on the exit face of the slab, whose Fourier decomposition can be written as follows (provided the thickness δ of the slab is very small):

$$f_{\text{out}}(t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \tilde{f}(\omega) e^{-i\omega(t - n'(\omega)/c\delta)} d\omega \quad [17]$$

In the latter, the real part of $n'(\omega)/c$ is the inverse of the light velocity in the medium, while its imaginary part takes into account the exponential damping of the wave. The output f_{out} thus appears as a causal

linear response with respect to f_{in} (since f_{out} “starts after” f_{in}). According to the general formula [10], the corresponding response function $\tilde{R}_\delta^{(c)}$ can be directly computed from eqns [16] and [17], which yields:

$$\tilde{R}_\delta^{(c)}(\omega^{(c)}) = e^{i\omega^{(c)}\hat{n}'(\omega^{(c)})\delta/c} \quad [18]$$

In view of the previous axiomatic analysis, $\tilde{R}_\delta^{(c)}$ has to be holomorphic and of moderate growth in \mathcal{I}_+ , and since this holds for all δ 's sufficiently small, it can be shown that the function $\hat{n}'(\omega^{(c)})$ itself is holomorphic and of moderate growth in \mathcal{I}_+ (no logarithmic singularity can be produced).

2. *Polarization of the medium produced by an electric field.* The dielectric polarization signal $P(t)$ produced at a point of a medium by an external electric field $E(t)$ is also a phenomenon of linear response which obeys the postulates (P1)–(P4); the corresponding formula [10] reads

$$\tilde{P}(\omega) = \chi'(\omega) \tilde{E}(\omega) \quad [19a]$$

where χ' is the complex dielectric susceptibility of the medium, which is related to n' by Maxwell's relation

$$\tilde{\chi}'(\omega) = \frac{[n'^2(\omega) - 1]}{4\pi} \quad [19b]$$

One thus recovers the fact that χ' admits an analytic continuation in \mathcal{I}_+ ; one can also show by a physical argument that $\tilde{\chi}'(\omega)$, and thereby $n'(\omega) - 1$, tends to zero as a constant divided by ω^2 when ω tends to infinity. This behavior at infinity extends to $\hat{n}'(\omega^{(c)}) - 1$ in \mathcal{I}_+ in view of the Phragmén–Lindelöf theorem, since \hat{n}' is known (from (1)) to be of moderate growth. This justifies the analytic background of Kramers–Krönig's relation.

From Relativistic QFT to the Dispersion Relations of Particle Physics: Historical Considerations and General Survey

In the quantum domain, the derivation of dispersion relations for the two-particle scattering (or collision) amplitudes of particle physics has represented, since 1956 and throughout the 1960s, an important conceptual progress for the theoretical treatment of that branch of physics. These phenomena are described in a quantum-theoretical framework in which the basic kinematical variables are the energies and momenta of the particles involved. These variables play the role of the frequency of light in the optical scattering phenomena. Moreover, since large energies and momenta are involved, which allow the occurrence of particle creation

according to the conservation laws of special relativity, it is necessary to use a relativistic quantum-mechanical framework. Around 1950, the success of the quantum electrodynamics formalism for computing the electron-photon, electron-electron, and electron-positron scattering amplitudes revealed the importance of the concept of relativistic quantum field for the understanding of particle physics. However, the methods of perturbation theory, which had ensured the success of quantum electrodynamics in view of the small value of the coupling parameter of that theory (namely the electric charge of the electron), were at that time inapplicable to the strong nuclear interaction phenomena of high-energy physics. This failure motivated an important school of mathematical physicists for working out a model-independent axiomatic approach of relativistic QFT (e.g., Lehmann, Symanzik, Zimmermann (1954), Wightman (1956), and Bogoliubov (1960); see *Axiomatic Quantum Field Theory*). Their main purpose was to provide a conceptually satisfactory treatment of relativistic quantum collisions, at least for the case of massive particles. Among various postulates expressing the invariance of the theory under the Poincaré group in an appropriate quantum-mechanical Hilbert-space framework, the approach basically includes a certain formulation of the principle of causality, called microcausality or local commutativity. This axiomatic approach of QFT was followed by a conceptually important variant, namely the algebraic approach to QFT (Haag, Kastler, Araki 1960), whose most important developments are presented in the book by Haag (1992) (see *Algebraic Approach to Quantum Field Theory*). From the historical viewpoint, and in view of the analyticity properties that they also generate, one can say that all these (closely related) approaches parallel the axiomatic approach of linear response phenomena with, of course, a much higher degree of complexity. In particular, the characterization of scattering (or collision) amplitudes in terms of appropriate structure functions of the basic quantum fields of the theory is a nontrivial preliminary step which was taken at an early stage of the theory under the name of “asymptotic theory and reduction formulae” (Lehmann, Symanzik, Zimmermann 1954–57, Haag–Ruelle 1962, Hepp 1965). There again, in the field-theoretical axiomatic framework, causality generates analyticity through Fourier–Laplace transformation, but several complex variables now play the role which was played by the complex frequency in the axiomatics of linear response phenomena: they are obtained by complexifying the relativistic energy-momentum variables of the (Fourier transforms of the) quantum fields involved in the high-energy

collision processes. In fact, the holomorphic functions which play the role of the causal response function $\tilde{R}(\omega)$ are the QFT structure functions or “Green functions in energy-momentum space.” The study of all possible analyticity properties of these functions resulting from the QFT axiomatic framework is called the analytic program (see *Scattering in Relativistic Quantum Field Theory: The Analytic Program*). The primary basic scope of the latter concerns the derivation of analyticity properties for the scattering functions of two-particle collision processes, which appears to be a genuine challenge for the following reason. The basic Einstein relation $E = mc^2$, which applies to all the incoming and outgoing particles of the collisions, operates as a geometrical constraint on the corresponding physical energy-momentum vectors: according to the Minkowskian geometry, the latter have to belong to mass hyperboloids, which define the so-called “mass shell” of the collision considered. It is on the corresponding complexified mass-shell manifold that the scattering functions are required to be defined as holomorphic functions. In the analytic program of QFT, the derivation of such analyticity domains and of corresponding dispersion relations in the complex plane of the squared total energy variable, s , of each given collision process then relies on techniques of complex geometry in several variables. As a matter of fact, the scattering amplitude is a function (or distribution) of two variables $F(s, t)$, where t is a second important variable, called the squared momentum transfer, which plays the role of a fixed parameter for the derivation of dispersion relations in the variable s . The value $t = 0$ corresponds to the special kinematical situation which has been described above (for the case of equal-mass particles Π_1 and Π_2) under the name of forward scattering and the variable s is a simple affine function of the energy ω of the colliding particle Π_1 in the laboratory Lorentz frame, (namely $s = 2m^2 + 2m\omega$ in the equal-mass case). It is for the corresponding scattering amplitude $T_0(\omega) \doteq F_0(s) \doteq F(s, t)|_{t=0}$ that a dispersion relation such as eqn [7] can be derived, although this derivation is far from being as simple as for the phenomena of linear response in classical physics: even in that simplest case, it already necessitates the use of analytic completion techniques in several complex variables. The first proof of this dispersion relation was performed by K Symanzik in 1956. In the case of general kinematical situations of measurements, the direction of observation of the scattered particle includes a nonzero angle with the incidence direction, which always corresponds to a negative value of t . The derivation of dispersion relations at fixed $t = t_0 < 0$, namely for the scattering amplitude

$F_{t_0}(s) \doteq F(s, t)|_{t=t_0}$ requires further arguments of complex geometry, and it is submitted to subtle limitations of the form $t_1 < t_0 \leq 0$, where t_1 depends on the mass spectrum of the particles involved in the theory. The first rigorous proof of dispersion relations at $t < 0$ was performed by N N Bogoliubov in 1960.

Three conceptually important features of the dispersion relations in particle physics deserve to be pointed out.

1. In comparison with the dispersion relations of classical optics, a feature which appears to be new is the so-called “crossing property,” which is characteristic of high-energy physics since it relies basically on the relativistic kinematics. According to that property, the boundary values of the analytic scattering function $\hat{F}_t(s)$ at positive and negative values of s from the respective half-planes $\text{Im } s > 0$ and $\text{Im } s < 0$ are interpreted, respectively, as the scattering amplitudes of two physically different collision processes, which are deduced from each other by replacing the incident particle by the corresponding antiparticle; one also says that “these two collision processes are related by crossing.” A typical example is provided by the proton–proton and proton–antiproton collisions, whose scattering amplitudes are therefore mutually related by the property of analytic continuation. This type of relationship between the values of the scattering function at positive and negative values of s generalizes in a nontrivial way the symmetry relation (S) satisfied by the forward scattering function $\hat{T}_0(\omega^{(c)})$ when each particle coincides with its antiparticle (see the second basic example above). No nontrivial crossing property holds in that special case and the fact that \hat{T}_0 is an even function of $\omega^{(c)}$ precisely expresses the identity of the two-collision processes related by crossing. In the general case, for $t = 0$ as well as for $t = t_0 < 0$ for any value of t_0 , the analyticity domain that one obtains for the scattering function is not the full cut-plane of s : in its general form, a “crossing domain” may exclude some bounded region B_{t_0} from the cut-plane, but it always contains an infinite region which is the exterior of a circle minus cuts along the two infinite parts of the real s -axis (Bros, Epstein, Glaser 1965): these cuts are along the physical regions of the two collision processes related by crossing. In that general case, the scattering function $\hat{F}_t(s)$ still satisfies what can be called a quasi-dispersion-relation, in which the right-hand side contains an additional Cauchy integral, taken along the boundary of B_t .

2. A second important feature concerns the behavior at large values of s of the scattering functions $\hat{F}_t(s)$ in their analyticity domain. As indicated in the presentation of the second basic

example, a “precise-increase” property was expected to be satisfied by the forward scattering amplitude $T_0(\omega)$ for ω (or s) tending to infinity. This “precise-increase” property implied the necessity of writing the corresponding dispersion relation [7] for the function $(T_0(\omega) - T_0(0))/\omega^2$: this is what one calls a “dispersion relation with a subtraction.” As a matter of fact, the existence of such restrictive bounds on the total cross sections at high energies had been discovered in 1961 by M Froissart: his derivation relied basically on the use of the unitarity of the scattering operator (expressing the quantum principle of conservation of probabilities), but also on a strong analyticity postulate for the scattering function not implied by the general field-theoretical approach (namely the Mandelstam domain of “double dispersion relations”). In the general framework of QFT, Froissart-type bounds appeared to be closely linked to a further nontrivial extension of the range of “admissible” values of t for which $\hat{F}_t(s)$ can be analytically continued in a cut-plane or crossing domain. In fact, the extension of this range to positive (i.e., “unphysical”) and even complex values of t , and as a second step the proof of Froissart-type bounds in $s(\log s)^2$ for $F_t(s)$ at all these admissible values of t , were performed in 1966 by A Martin. They rely on a subtle conspiracy of the analyticity properties deduced from the QFT axiomatic framework and of positivity and unitarity properties expressing the basic Hilbertian structure of the quantum collision theory. The consequence of these bounds on the exact form of the dispersion relations is that, as in formula [7] of the case $t = 0$, it is justified to write a (the so-called “subtracted”) dispersion relation for $(F_t(s) - F_t(0) - sF'_t(0))/s^2$: for the general case when the crossing property replaces the symmetry (S), such a dispersion relation involves two subtractions (since $F'_t(0) \neq 0$). Detailed information concerning the interplay of analyticity and unitarity on the mass shell and the derivation of refined forms of dispersion relations and various boundedness properties for the scattering functions are given in the book by Martin (1969).

3. Constraints imposed by dispersion relations and experimental checks. The conceptual importance of dispersion relations incorporating the above features (1) and (2) is displayed by such spectacular application as the relationship between the high-energy behaviors of proton–proton and proton–antiproton cross sections. Even though the closest forms of relationship between these cross sections (e.g., the existence of equal high-energy limits) necessitate for their proof some extra assumption concerning, for instance, the behavior

of the ratio between the dispersive and absorptive parts of the forward scattering amplitude, one can speak of an actual model-independent implication of general QFT that imposes nontrivial constraints on phenomena. Otherwise stated, checking experimentally the previous type of relationship up to the limits of high energies imposed by the present technology of accelerators constitutes an indirect, but important test of the validity of the general principles of QFT.

As a matter of fact, it has also appeared frequently in the literature of high-energy physics during the last 40 years that the Froissart bound by itself was considered as a key criterion to be satisfied by any sensible phenomenological model in particle physics. As already stated above, the Froissart bound is one of the deepest consequences of the analytic program of general QFT, since its derivation also incorporates in the most subtle way the quantum principle of probability conservation. Would it be only for the previous basic results, the derivation of dispersion relations (and, more generally, the results of the analytic program) in QFT appear as an important conceptual bridge between a fundamental theoretical framework of relativistic quantum physics and the phenomenology of high-energy particle physics.

Basic Concepts and Main Steps in the QFT Derivation of Dispersion Relations

The rest of this article outlines the derivation of the analytic background of dispersion relations for the forward scattering amplitudes in the framework of axiomatic QFT. After a brief introduction on relativistic scattering processes and the problematics of causality in particle physics, it gives an account of the Wightman axioms and the simplest reduction formula which relates the forward scattering amplitude to a retarded product of the field operators. Then it describes how the latter can be used for justifying a certain type of analyticity domain for the forward scattering functions, namely a crossing domain or in the best cases a cut-plane in the squared energy variable s . This is the basic result that allows one to write dispersion relations (or quasi-dispersion-relations) at $t=0$; the exact form of the latter, including at most two subtractions, relies on the use of Hilbertian positivity and of the unitarity of the scattering operator.

Relativistic Quantum Scattering as a Phenomenon of Linear Response

Collisions of quantum particles may be seen as phenomena of linear response, but in a way which

differs greatly from what has been previously described.

Particles in Minkowskian geometry Each state of a relativistic classical particle with mass m is characterized by its energy-momentum vector or 4-momentum $p = (p_0, \mathbf{p})$ satisfying the mass-shell condition $p^2 \doteq p_0^2 - \mathbf{p}^2 = m^2$ (in units such that $c=1$). In view of the condition of positivity of the energy $p_0 > 0$ the “physical mass shell” thus coincides with the positive sheet H_m^+ of the mass hyperboloid H_m with equation $p^2 = m^2$.

The set of all energy-momentum configurations characterizing the collisions of two relativistic classical particles with initial (resp. final) 4-momenta p_1, p_2 (resp. p'_1, p'_2) is the mass-shell manifold \mathcal{M} defined by the conditions

$$p_i^2 = m^2, \quad p_i'^2 = m^2, \quad p_{i,0} > 0, \quad p'_{i,0} > 0, \quad i = 1, 2$$

$$p_1 + p_2 = p'_1 + p'_2$$

where the latter equation expresses the relativistic law of total energy-momentum conservation. \mathcal{M} is an eight-dimensional manifold, invariant under the (six-dimensional) Lorentz group: the orbits of this group that constitute a foliation of \mathcal{M} are parametrized by two variables, namely the squared total energy $s = (p_1 + p_2)^2 = (p'_1 + p'_2)^2$ and the squared momentum transfer $t = (p_1 - p'_1)^2 = (p_2 - p'_2)^2$ (or $u = (p_1 - p'_2)^2 = 4m^2 - s - t$). In these variables, called the Mandelstam variables, the “physical region” Φ of the collision is represented by the set of pairs (s, t) (or triplets (s, t, u) with $s + t + u = 4m^2$) such that $t \leq 0, u \leq 0$, and therefore $s \geq 4m^2$.

Correspondingly, each state of a relativistic quantum particle with mass m is characterized by a wave packet $\hat{f}(p)$ on H_m^+ , which is an element of unit norm of $L_2(H_m^+, \mu_m(p))$, with $\mu_m(p) = d\mathbf{p}/(p^2 + m^2)^{1/2}$. In Minkowskian spacetime with coordinates $x = (x_0, \mathbf{x})$, any such state is represented by a wave function $f(x)$ whose Fourier transform is the tempered distribution (with support in H_m^+) $\hat{f}(p) \times \delta(p^2 - m^2)$: $f(x)$ is a positive-energy solution of the Klein-Gordon equation $(\partial^2/\partial x_0^2 - \Delta_{\mathbf{x}} + m^2)f(x) = 0$. A free two-particle state is a symmetric wave packet $\hat{f}(p_1, p_2)$ on $H_m^+ \times H_m^+$ in the Hilbert space $L_2(H_m^+ \times H_m^+, \mu_m \otimes \mu_m)$.

Scattering kernels as response kernels: distribution character

While the input to be considered is a free wave packet $\hat{f}_{\text{in}}(p_1, p_2)$ on $H_m^+ \times H_m^+$, representing the preparation of an initial two-particle state, the output corresponds to the detection of a final two-particle state also characterized by a wave packet $\hat{g}_{\text{out}}(p'_1, p'_2)$ on $H_m^+ \times H_m^+$. In quantum mechanics, linearity is linked to the “superposition principle” of states,

which allows one to state that collisions are described by a certain bilinear form $(\hat{f}_{\text{in}}, \hat{g}_{\text{out}}) \rightarrow S(\hat{f}_{\text{in}}, \hat{g}_{\text{out}})$, called the “scattering matrix.” This bilinear form is bicontinuous with respect to the Hilbertian norms of the wave packets, and it then results from the Schwartz nuclear theorem that it is represented by a distribution kernel $S(p_1, p_2; p'_1, p'_2)$, namely a tempered distribution with support contained in \mathcal{M} , in such a way that (formally)

$$S(\hat{f}_{\text{in}}, \hat{g}_{\text{out}}) = \int \hat{f}_{\text{in}}(p_1, p_2) \overline{\hat{g}_{\text{out}}(p'_1, p'_2)} S(p_1, p_2; p'_1, p'_2) \times \mu_m(p_1) \mu_m(p_2) \mu_m(p'_1) \mu_m(p'_2) \quad [20]$$

If there were no interaction, $S(\hat{f}_{\text{in}}, \hat{g}_{\text{out}})$ would reduce to the Hilbertian scalar product $\langle \hat{g}_{\text{out}}, \hat{f}_{\text{in}} \rangle$ in $L_2(H_m^+ \times H_m^+; \mu_m \otimes \mu_m)$ and the corresponding kernel S would be the identity kernel

$$I(p_1, p_2; p'_1, p'_2) = \frac{1}{2} [\delta(p_1 - p'_1) \delta(p_2 - p'_2) + \delta(p_1 - p'_2) \delta(p_2 - p'_1)]$$

In the general case, the interaction is therefore described by the scattering kernel $T(p_1, p_2; p'_1, p'_2) \doteq S(p_1, p_2; p'_1, p'_2) - I(p_1, p_2; p'_1, p'_2)$. The action of T as a bilinear form (defined in the same way as the action of S in eqn [20]) may be seen as the quantum analog of the classical response formula [10]. Note, however, the difference in the mathematical treatment of the output: instead of being considered as the direct response (\hat{f}_{out}) to the input, it is now explored by Hilbertian duality in terms of detection wave packets \hat{g}_{out} , in conformity with the principles of quantum theory. Finally, in view of the invariance of the collision process under the Lorentz group, the scattering kernel T is constant along the orbits of this group in \mathcal{M} and it then defines a distribution $F(s, t) \doteq T(p_1, p_2; p'_1, p'_2)$ with support in the physical region Φ : this is what is called the scattering amplitude.

What becomes of causality? One can show that the positive-energy solutions of the Klein–Gordon equation cannot vanish in any open set of Minkowski spacetime; they necessarily spread out in the whole spacetime. This makes it impossible to formulate a causality condition comparable to eqn [9] in terms of the spacetime wave functions \hat{f}_{in} and \hat{g}_{out} corresponding to the input and output wave packets $\hat{f}_{\text{in}}, \hat{g}_{\text{out}}$. In this connection, it is, however, appropriate to note that (after various attempts of “weak causality conditions”) a certain condition called “macrocausality” (Iagolnitzer and Stapp 1969; see the book by Iagolnitzer (1992)) has been shown to be equivalent to some local properties of analyticity

of the scattering kernel T ; but it is not our purpose to develop that point here for two reasons: (1) the interpretation of that condition is rather involved, because it integrates a very weak form of causality together with the spatial short-range character of the strong nuclear interactions between the elementary particles; (2) the domains of analyticity obtained are by far too small with respect to those necessary for writing dispersion relations. The reason for this failure is that the scattering kernel only represents an asymptotic quantum observable, in the sense that it is intended to describe observations far apart from the extremely small spacetime region where the particles strongly interact, namely in regions where this interaction is asymptotically small. Although well adapted to what is actually observed in the detection experiments, the concept of scattering kernel is not sufficient for describing the fundamental interactions of physics: it must be enriched by other theoretical concepts which might explicitly take into account the microscopic interactions in spacetime. This motivates the introduction of quantum fields as basic quantities in particle physics.

Relativistic Quantum Fields: Microcausality and the Retarded and Advanced Kernels; Analyticity in Complex Energy–Momentum Space

By an idealization of the concept of quantum electromagnetic field and a generalization to all types of microscopic interactions of matter, one considers that all the phenomena involving such interactions can be described by fields $\Phi_i(x)$, whose amplitude can, in principle, be measured in arbitrarily small regions of Minkowski spacetime. In the quantum framework, one is thus led to the notion of local observable \mathcal{O} (emphasized as a basic concept in the axiomatic approach of Araki, Haag, and Kastler). In the Wightman field-theoretical framework, a local observable corresponds to the measuring process of a ponderated average of a field $\Phi_i(x)$ of the form $\mathcal{O} \doteq \Phi_i[f] = \int \Phi_i(x) f(x) dx$. In the latter, $f(x)$ denotes a smooth real-valued test-function with (arbitrary) compact support K in spacetime; the observable \mathcal{O} is then said to be localized in K . Each observable $\mathcal{O} = \Phi_i(f)$ has to be a self-adjoint (unbounded) operator acting in (a dense domain of) the Hilbert space \mathcal{H} generated by all the states of the system of fundamental fields $\{\Phi_i\}$; therefore, the correct mathematical concept of relativistic quantum field $\Phi(x)$ is an “operator-valued tempered distribution on Minkowski spacetime.” Here the additional “temperateness assumption” is a convenient technical assumption which in particular allows the passage to the energy–momentum space by making use of the Fourier transformation.

In this QFT framework, it is natural to express a certain form of causality by assuming that two observables $\Phi(f)$ and $\Phi(f')$ commute if the supports of f and f' are spacelike-separated regions in spacetime, which means that no signal with velocity smaller or equal to the velocity of light can propagate from either one of these regions to the other. This expresses the idea that these two observables should be independent, that is, “compatible as quantum observables.” This postulate is equivalent to the following condition, called microcausality or local commutativity, and understood in the sense of operator-valued tempered distributions:

$$[\Phi(x_1), \Phi(x'_1)] = 0, \quad \text{for } (x_1 - x'_1)^2 < 0 \quad [21]$$

where $(x_1 - x'_1)^2$ is the squared Minkowskian pseudonorm of $x = x_1 - x'_1 = (x_0, \mathbf{x})$, namely $x^2 = x_0^2 - \mathbf{x}^2$. It follows that for every admissible pair of states Ψ, Ψ' in \mathcal{H} , the tempered distribution

$$C_{\Psi, \Psi'}(x_1, x'_1) \doteq \langle \Psi, [\Phi(x_1), \Phi(x'_1)] \Psi' \rangle \quad [22]$$

has its support contained in the union of the sets $\mathcal{V}^+ : x_1 - x'_1 \in \overline{V^+}$ and $\mathcal{V}^- : x_1 - x'_1 \in \overline{V^-}$, where $\overline{V^+}$ and $\overline{V^-}$ are, respectively, the closures of the forward and backward cones $V^+ \doteq \{x = (x_0, \mathbf{x}); x_0 > |\mathbf{x}|\}$, $V^- \doteq -V^+$ in Minkowski spacetime. It is always possible to decompose the previous distribution as

$$C_{\Psi, \Psi'}(x_1, x'_1) = R_{\Psi, \Psi'}(x_1, x'_1) - A_{\Psi, \Psi'}(x_1, x'_1) \quad [23]$$

in such a way that the supports of the distributions $R_{\Psi, \Psi'}(x_1, x'_1)$ and $A_{\Psi, \Psi'}(x_1, x'_1)$ belong, respectively, to \mathcal{V}^+ and \mathcal{V}^- . $R_{\Psi, \Psi'}$ and $A_{\Psi, \Psi'}$ are called, respectively, retarded and advanced kernels and they are often formally expressed (for convenience) as follows:

$$\begin{aligned} R_{\Psi, \Psi'}(x_1, x'_1) &= \theta(x_{1,0} - x'_{1,0}) C_{\Psi, \Psi'}(x_1, x'_1) \\ A_{\Psi, \Psi'}(x_1, x'_1) &= -\theta(x_{1,0} - x'_{1,0}) C_{\Psi, \Psi'}(x_1, x'_1) \end{aligned}$$

in terms of the Heaviside step function $\theta(t)$ of the time-coordinate difference $t = x_{1,0} - x'_{1,0}$. For every pair (Ψ, Ψ') , $R_{\Psi, \Psi'}(x_1, x'_1)$ appears as a relativistic generalization of the retarded kernel $R(t - t')$ of eqn [10]: its support property in spacetime, similar to the support property of R in time, expresses a relativistic form of causality, or “Einstein causality.”

There exists a several-variable extension of the theory of Fourier–Laplace transforms of tempered distributions which is based on a formula similar to eqn [11]. We introduce the vector variables $X = (x_1 + x'_1)/2$, $x = x_1 - x'_1$ and a complex 4-momentum $k = p + iq = (k_0, \mathbf{k})$ as the conjugate

vector variable of x with respect to the Minkowskian scalar product $k \doteq k_0 x_0 - \mathbf{k} \cdot \mathbf{x}$, and we define

$$\tilde{R}_{\Psi, \Psi'}^{(c)}(k, X) = \int_{\overline{V^+}} R_{\Psi, \Psi'}\left(X + \frac{x}{2}, X - \frac{x}{2}\right) e^{ik \cdot x} dx \quad [24]$$

Since $q \cdot x > 0$ for all pairs (q, x) such that $q \in V^+$, $x \in \overline{V^+}$, it follows that $\tilde{R}_{\Psi, \Psi'}^{(c)}(k, X)$ is holomorphic with respect to k in the domain \mathcal{T}^+ containing all $k = p + iq$ such that q belongs to V^+ . Moreover, in the limit $q \rightarrow 0$ this holomorphic function tends (in the sense of distributions) to the Fourier transform $\tilde{R}_{\Psi, \Psi'}(p, X)$ of $R_{\Psi, \Psi'}(X + x/2, X - x/2)$ with respect to x . The domain \mathcal{T}^+ , which is called the “forward tube,” is the analog of the domain \mathcal{I}_+ of the ω -plane; bounds of moderate type comparable to those of [12] apply to the holomorphic function $\tilde{R}_{\Psi, \Psi'}^{(c)}$ in \mathcal{T}^+ . Similarly, the advanced kernel $A_{\Psi, \Psi'}(X + x/2, X - x/2)$ admits a Fourier–Laplace transform $\tilde{A}_{\Psi, \Psi'}^{(c)}(k, X)$, which is holomorphic and of moderate growth in the “backward tube” \mathcal{T}^- containing all $k = p + iq$ such that q belongs to V^- . In view of [23], the Fourier transform $\tilde{C}_{\Psi, \Psi'}(p, X)$ of $C_{\Psi, \Psi'}(X + x/2, X - x/2)$ then appears as the difference between the boundary values of $\tilde{R}_{\Psi, \Psi'}^{(c)}$ and $\tilde{A}_{\Psi, \Psi'}^{(c)}$ on the reals (from the respective domains \mathcal{T}^+ and \mathcal{T}^-).

The Field-Theoretical Axiomatic Framework and the Passage from the Structure Functions of QFT to the Scattering Kernels (Case of Forward Scattering)

The postulates (Wightman axioms) Apart from the causality postulate, which we have already presented above in view of its distinguished role for generating analyticity properties in complex energy–momentum space, the field-theoretical axiomatic approach to collision theory is based on the following postulates (for all the fundamental developments of axiomatic field theory, the interested reader may consult the books by Streater and Wightman (1980) and by Jost (1965); see Axiomatic Quantum Field Theory).

1. There exists a unitary representation $g \rightarrow U(g)$ of the Poincaré group G in the Hilbert space of states \mathcal{H} ; in this representation, the abelian subgroup of translations of space and time has a Lie algebra whose generators are interpreted as the four self-adjoint (commuting) operators P_μ of total energy–momentum of the system.
2. The quantum field operators $\Phi(x)$ transform covariantly under that representation; in the simplest case of scalar fields (considered here), $\Phi(gx) = U(g)\Phi(x)U(g^{-1})$.
3. There exists a unique state Ω , called the vacuum, such that the action of all polynomials of field operators on Ω generates a dense subset of \mathcal{H} ;

moreover, Ω is assumed to be invariant under the representation \mathcal{U} of G , and thereby such that $P_\mu \Omega = 0$.

4. Spectral condition or positivity of energy in all physical states. The joint spectrum Σ of the operators P_μ is contained in the closed forward cone $\overline{V^+}$ of energy-momentum space. In order to perform the collision theory of massive particles, one needs a more detailed "mass-gap assumption": Σ is the union of the origin O , of one or several positive sheets of hyperboloid $H_{m_i}^+$ and of a region V_M^+ defined by the conditions $p^2 \geq M^2, p_0 > 0$, with M larger than all the m_i .

The Hilbert space \mathcal{H} is correspondingly decomposed as the direct sum of the vacuum subspace (or zero-particle subspace) generated by Ω , of subspaces of stable one-particle states with masses m_i isomorphic to $L_2(H_{m_i}^+, \mu_{m_i})$, and of a remaining subspace \mathcal{H}' . As a result of the construction of "asymptotic states," \mathcal{H}' can be shown to contain two subspaces \mathcal{H}'_{in} and $\mathcal{H}'_{\text{out}}$, generated, respectively, by N -particle incoming states (with N arbitrary and ≥ 2) and by N -particle outgoing states. The collision operator S is then defined as the partially isometric operator from $\mathcal{H}'_{\text{out}}$ onto \mathcal{H}'_{in} , which maps a reference basis of outgoing states onto the corresponding basis of incoming states.

An independent postulate: asymptotic completeness (see *Scattering, Asymptotic Completeness and Bound States and Scattering in Relativistic Quantum Field Theory: Fundamental Concepts and Tools*) The theory is said to satisfy the property of asymptotic completeness if all the states of \mathcal{H} can be interpreted as superpositions of various N -particle states (either in the incoming or in the outgoing state basis), namely if one has $\mathcal{H}' = \mathcal{H}'_{\text{in}} = \mathcal{H}'_{\text{out}}$. This property is not implied by the previous postulates on quantum fields, but its physical interpretation and its role in the analytic program are of primary importance (see *Scattering in Relativistic Quantum Field Theory: The Analytic Program*). Let us simply note here that asymptotic completeness implies as a by-product the unitarity property of the collision operator S on the full Hilbert space \mathcal{H}' (i.e., $SS^* = S^*S = I$).

Connection between retarded kernel and scattering kernel for the forward scattering case; a simple "reduction formula" We consider the scattering of a particle Π_1 with mass m_1 on a target consisting of a particle Π_2 with mass m_2 and denote by $T(p_1, p_2; p'_1, p'_2)$ the corresponding scattering kernel (defined similarly as for the case of equal-mass

particles considered earlier). Equations [22]–[24] are then applied to the case when Ψ and Ψ' coincide with a one-particle state of Π_2 at rest, namely with 4-momentum $p_2 = p'_2$ along the time axis: $p_2 = ((p_2)_0, 0), (p_2)_0 = m_2$. This describes in a simple way the case of forward scattering, since in view of the energy-momentum conservation law $p_1 + p_2 = p'_1 + p'_2$, the choice $p_2 = p'_2$ also implies that $p_1 = p'_1$. (The possibility of restricting the distribution $T(p_1, p_2; p'_1, p'_2)$ to such fixed values of the energy-momenta is shown to be mathematically well justified). The advantage of this simple case is that the corresponding kernels [22], [23] of (x_1, x'_1) are invariant under spacetime translations and therefore depend only on x (and not on X). We can thus rewrite eqns [22], [23] with simplified notations as follows:

$$\begin{aligned} C_{p_2}(x) &\doteq \langle p_2, \left[\Phi\left(\frac{x}{2}\right), \Phi\left(-\frac{x}{2}\right) \right] p_2 \rangle \\ &= R_{p_2}(x) - A_{p_2}(x) \end{aligned} \quad [25]$$

which can be shown to give correspondingly by Fourier transformation

$$\begin{aligned} \tilde{C}_{p_2}(p) &= \langle p_2, \tilde{\Phi}(p) \tilde{\Phi}(-p) p_2 \rangle - \langle p_2, \tilde{\Phi}(-p) \tilde{\Phi}(p) p_2 \rangle \\ &= \tilde{R}_{p_2}(p) - \tilde{A}_{p_2}(p) \end{aligned} \quad [26]$$

If the particle Π_1 appears in the asymptotic states of the field Φ , the scattering kernel $T(p_1, p_2; p'_1, p'_2)$ is then given in the forward configurations $p_1 = p'_1 \in H_{m_1}^+, p_2 = p'_2 \in H_{m_2}^+$, by the following reduction formula in which $s = (p_1 + p_2)^2$:

$$\begin{aligned} F_0(s) &= T(p_1, p_2; p_1, p_2) \\ &= [(p_1^2 - m_1^2) \tilde{R}_{p_2}(p_1)]|_{H_{m_1}^+} \end{aligned} \quad [27]$$

Analyticity Domains in Energy-Momentum Space: From the "Primitive Off-Shell Domains" of QFT to the Crossing Manifolds on the Mass Shell

For simplicity, we shall restrict ourselves to the consideration of forward scattering amplitudes, namely to the derivation of crossing analyticity domains and (quasi-)dispersion relations at $t = 0$ for two-particle collision processes of the form $\Pi_1 + \Pi_2 \rightarrow \Pi_1 + \Pi_2$, Π_1 and Π_2 being given massive particles with arbitrary spins and charges.

The holomorphic function $H_{p_2}(k)$ and its primitive domain D . Nontriviality of dispersion relations for the scattering amplitudes As suggested by eqn [24], we can exploit the analyticity properties of the Fourier-Laplace transforms of the retarded and advanced kernels R_{p_2} and A_{p_2} : in fact, $\tilde{R}_{p_2}(p)$ and

$\tilde{A}_{p_2}(p)$ are, respectively, the boundary values of the holomorphic functions

$$\begin{aligned}\tilde{R}_{p_2}^{(c)}(k) &= \int_{V^+} R_{p_2}(x) e^{ik \cdot x} dx \\ \tilde{A}_{p_2}^{(c)}(k) &= \int_{V^-} A_{p_2}(x) e^{ik \cdot x} dx\end{aligned}\quad [28]$$

from the corresponding domains T^+ and T^- . According to the reduction formula [27], it is appropriate to consider correspondingly the functions $H_{p_2}^+(k) \doteq (k^2 - m_1^2)\tilde{R}_{p_2}^{(c)}(k)$ and $H_{p_2}^-(k) \doteq (k^2 - m_1^2)\tilde{A}_{p_2}^{(c)}(k)$, which are also, respectively, holomorphic in T^+ and T^- . Then the forward scattering amplitude $F_0(s) = F(s, 0) = T(p_1, p_2; p_1, p_2)$ appears as the restriction to the hyperboloid sheet $p \in H_{m_1}^+$ of the boundary value $H_{p_2}^+(p)$ of $H_{p_2}^+(k)$ on the reals.

Moreover, it can be seen that the two boundary values $H_{p_2}^+(p) = (p^2 - m_1^2)\tilde{R}_{p_2}(p)$ and $H_{p_2}^-(p) = (p^2 - m_1^2)\tilde{A}_{p_2}(p)$ coincide as distributions in the region

$$\mathcal{R} = \{p \in \mathbb{R}^4; (p + p_2)^2 < (m_1 + m_2)^2; (p - p_2)^2 < (m_1 + m_2)^2\} \quad [29]$$

This follows from the intermediate expression in eqn [26] and from the fact that a state of the form $(p^2 - m_1^2)\Phi(\pm p)p_2 >$ is a state of energy-momentum $\pm p + p_2$ and therefore vanishes (in view of the spectral condition) if $(\pm p + p_2)^2 < (m_1 + m_2)^2$ (here we also use a simplifying assumption according to which no one-particle bound state is present in this channel).

The situation obtained concerning the holomorphic functions $H_{p_2}^+(k)$ and $H_{p_2}^-(k)$ parallels (in complex dimension four) the case of a pair of holomorphic functions in the upper and lower half-planes whose boundary values on the reals coincide on a certain interval playing the role of \mathcal{R} . As in this one-dimensional case there is a theorem, called the “edge-of-the-wedge theorem” (see below), which implies that $H_{p_2}^+(k)$ and $H_{p_2}^-(k)$ have a common analytic continuation $H_{p_2}(k)$: this function is holomorphic in a domain D which is the union of T^+ , T^- and of a complex neighborhood of \mathcal{R} ; D is called the primitive domain of $H_{p_2}(k)$.

Moreover, it follows from the postulate of invariance of the field $\Phi(x)$ under the action of the Poincaré group (see postulate (2)) that the holomorphic function $H_{p_2}(k)$ only depends of the two complex variables $\zeta = k^2 (= k_0^2 - k^2)$ and $k \cdot p_2$ or equivalently $s = (k + p_2)^2 = \zeta + m_2^2 + 2k \cdot p_2$; it thus defines a corresponding holomorphic function $\hat{H}_{p_2}(\zeta, s) \doteq H_{p_2}(k)$ in the image of D in these variables.

In view of the reduction formula [27], the scattering function $\hat{F}_0(s)$ should appear as the

restriction of the holomorphic function $\hat{H}_{p_2}(\zeta, s)$ to the physical mass-shell value $\zeta = m_1^2$. However, it turns out that the section of D by the complex mass-shell manifold $\mathcal{M}^{(c)}$ with equation $k^2 = m_1^2$ is empty: this geometrical fact is responsible for the nontriviality of the proof of dispersion relations for the physical quantity $\hat{F}_0(s)$ on the mass shell. In fact, the tube $T^+ \cup T^-$ which constitutes the basic part of the domain D and is given by the field-theoretical microcausality postulate, is a “purely off-shell” complex domain, as it can be easily checked: if a complex point $k = p + iq$ is such that $q^2 > 0$, the corresponding squared mass $\zeta = k^2 = p^2 - q^2 + 2ip \cdot q$ is real if and only if $p \cdot q = 0$, which implies $p^2 < 0$ (i.e., p spacelike) and therefore $\zeta = p^2 - q^2 < 0$.

“Off-shell dispersion relations” as a first step The starting point, which is easy to obtain from the domain D , is the analyticity of the holomorphic function $\hat{H}_{p_2}(\zeta, s)$ in a cut-plane of the variable s for all negative values of the squared mass variable ζ . This cut-plane Δ_ζ is always the complement in \mathbb{C} (i.e., the complex s -plane) of the union of the s -cut (s real $\geq (m_1 + m_2)^2$) and of the u -cut ($u = 2\zeta + 2m_2^2 - s$ real $\geq (m_1 + m_2)^2$). This analyticity property thus justifies “off-shell dispersion relations” at fixed negative values of ζ for the field-theoretical structure function $\hat{H}_{p_2}(\zeta, s)$.

The latter property and the subsequent analysis concerning the process of analytic continuation of \hat{H}_{p_2} to positive values of ζ will be more easily understood geometrically if one reduces the complex space of k to a two-dimensional complex space, which is legitimate in view of the equality $H_{p_2}(k) = \hat{H}_{p_2}(\zeta, s)$.

Having chosen the k_0 -axis along p_2 , we reduce the orthogonal space coordinates \mathbf{k} of k to the radial variable k_r . One thus gets the following expressions of the variables ζ and s (resp. u):

$$\begin{aligned}\zeta &= k_0^2 - k_r^2, \quad s = \zeta + m_2^2 + 2m_2 k_0 \\ (\text{resp. } u &= \zeta + m_2^2 - 2m_2 k_0)\end{aligned}$$

Then we can write $\hat{H}_{p_2}(\zeta, s) \doteq H_{p_2}(k_0, k_r) = H_{p_2}(k_0, -k_r)$, and describe the image D_r of the domain D in the variables $k = (k_0, k_r) = p + iq$ as $T_r^+ \cup T_r^- \cup \mathcal{N}(\mathcal{R}_r)$, where:

1. T_r^\pm is defined by the condition $q^2 \doteq q_0^2 - q_r^2 > 0$, $q_0 > 0$ or $q_0 < 0$,
2. \mathcal{N} is a complex neighborhood of the real region \mathcal{R}_r defined as follows. Let h_s^+, h_u^- be the two branches of hyperbolae with respective equations:

$$\begin{aligned}h_s^+ : (p_0 + m_2)^2 - p_r^2 &= (m_1 + m_2)^2, \quad p_0 + m_2 > 0 \\ h_u^- : (p_0 - m_2)^2 - p_r^2 &= (m_1 + m_2)^2, \quad p_0 - m_2 < 0\end{aligned}$$

Then \mathcal{R}_r is the intersection of the region situated below h_s^+ and of the region situated above h_u^- .

Let us now consider any complex hyperbola $h^{(c)}[\zeta]$ with equation $k^2 \doteq k_0^2 - k_r^2 = \zeta$. On such a complex curve either one of the variables k_0 or s or u is a good parameter for holomorphic functions which are even in k_r , like $H_{p_2}(k_0, k_r)$. If ζ is real, any complex point $k = p + iq$ of $h^{(c)}[\zeta]$ is such that p^2 and q^2 have opposite signs (since $p \cdot q = 0$). Therefore, the sign of q^2 is always opposite to the sign of $\zeta (= p^2 - q^2)$: if ζ is negative, all the complex points of $h^{(c)}[\zeta]$ thus belong to $T_r^+ \cup T_r^-$; the union of all these points with the real points of $h^{(c)}[\zeta]$ in \mathcal{R}_r is therefore a subset of D_r , which is represented in the complex plane of s by the cut-plane Δ_ζ . The function $\hat{H}_{p_2}(\zeta, s)$ is therefore analytic (and univalent) in Δ_ζ for each $\zeta < 0$. Moreover, the existence of moderate bounds of type [12] on H_{p_2} in D (resulting from the temperateness assumption) then implies the validity of dispersion relations (with subtractions) for $\hat{H}_{p_2}(\zeta, s)$ in Δ_ζ .

The problem of analytic completion to the complex mass-shell hyperbola $h^{(c)}[m_1^2]$: what is provided by the Jost-Lehmann-Dyson domain A basic fact in complex geometry in n variables, with $n \geq 2$, is the existence of a distinguished class of domains, called holomorphy domains: for each domain \mathcal{U} in this class, there exists at least one function which is holomorphic in \mathcal{U} and cannot be analytically continued at any point of the boundary of \mathcal{U} . In one dimension, every domain is a holomorphy domain. In dimension larger than one, a general domain \mathcal{U} is not a holomorphy domain, but it admits a holomorphy envelope $\hat{\mathcal{U}}$, which is a holomorphy domain containing \mathcal{U} , such that every function holomorphic in \mathcal{U} admits an analytic continuation in $\hat{\mathcal{U}}$.

It turns out that the domain D_r considered above in the last subsection) is not a holomorphy domain; its holomorphy envelope \hat{D}_r (obtained geometrically by Bros, Messiah, and Stora in 1961) coincides with a domain introduced by Jost-Lehmann (1957) and Dyson (1958) by methods of wave equations. This domain can be characterized as the union of D_r with all the complex points of all the hyperbolae with equations $(k_0 - a)^2 - (k_r - b)^2 = c^2$ (for all a, b, c real, including the complex straight lines for which $c = 0$) whose both branches have a nonempty intersection with the real region \mathcal{R}_r .

In particular, one easily sees that all the hyperbolae $h^{(c)}[\zeta]$ with $0 \leq \zeta < m_1^2$ belong to the previous class. It follows that for any ζ in this positive interval, the function $\hat{H}_{p_2}(\zeta, s)$ can still be

analytically continued as a holomorphic function of s in the cut-plane Δ_ζ and thereby satisfies the corresponding dispersion relations.

The physical mass shell hyperbola $h^{(c)}[m_1^2]$ thus appears as a limiting case of the previous family (for ζ tending to m_1^2 from below). The analyticity of $\hat{H}_{p_2}(m_1^2, s)$ in $\Delta_{m_1^2}$ can then be justified provided one knows that this function is analytic at at least one point of $\Delta_{m_1^2}$: but this additional information results from a more thorough exploitation of the analyticity properties resulting from the QFT postulates. This will be now briefly outlined below.

Further information coming from the four-point function in complex momentum space It is possible to obtain further analyticity properties of $\hat{H}_{p_2}(\zeta, s) \doteq H_{p_2}(k)$ by considering the latter as the restriction to the submanifold $k_1 = -k_3 = k$; $k_2 = -k_4 = p_2$ of a master analytic function $H_4(k_1, k_2, k_3, k_4)$, called the four-point function of the field Φ in complex energy-momentum space (see Scattering in Relativistic Quantum Field Theory: The Analytic Program). This function is holomorphic in a well-defined primitive domain D_4 of the linear submanifold $k_1 + k_2 + k_3 + k_4 = 0$. It is then possible to compute some local parts situated near the reals of the holomorphy envelope of D_4 , which implies, as a by-product, that the function $\hat{H}_{p_2}(\zeta, s)$ can be analytically continued in a set Σ of the form

$$\Sigma = \{(\zeta, s); \zeta \in \delta, s \in \mathcal{V}_{s_1}(\zeta)\} \cup \{(\zeta, s); \zeta \in \delta, u = 2\zeta + 2m_2^2 - s \in \mathcal{V}_{u_1}(\zeta)\} \quad [30]$$

with the following specifications:

1. δ is a domain in the ζ -plane, which is a complex neighborhood of a real interval of the form $-a < \zeta < M_1^2$; here M_1 denotes a spectral mass threshold in the theory such that $M_1 > m_1$;
2. for each ζ , $\mathcal{V}_{s_1}(\zeta)$ (resp. $\mathcal{V}_{u_1}(\zeta)$) is a cut-neighborhood in the s -plane of the real half-line $s > s_1$ (resp. of the half-line $u = 2\zeta + 2m_2^2 - s$ real $> u_1$); s_1 and u_1 denote appropriate real numbers independent of ζ .

The final analytic completion: crossing domains on $h^{(c)}[m_1^2]$. Dispersion relations for $\pi_0\text{--}\pi_0$ meson scattering and “quasi-dispersion-relations” for proton-proton scattering We now wish to describe briefly the final step of analytic completion, which displays the existence of a “quasi-cut-plane domain” in s for the function $\hat{H}_{p_2}(m_1^2, s)$, even in the more general case when the s -cut and u -cut are associated with different scattering channels, whose respective mass thresholds $s = M_{12}^2$ and $u = M_{12}^2$ are unequal.

This general situation may occur as soon as one charged particle Π_1 of the s -channel is replaced by the corresponding antiparticle $\bar{\Pi}_1$ in the u -channel, in contrast with the case of neutral particles (like the π_0 meson) which coincide with their own antiparticles. Here it is important to note that the two real branches $h^+[m_1^2]$ and $h^-[m_1^2]$ of the mass shell hyperbola $h^{(c)}[m_1^2]$ correspond, respectively, to the physical region of the “direct scattering channel” of the reaction $\Pi_1 + \Pi_2 \rightarrow \Pi_1 + \Pi_2$ with squared total energy s , and to the physical region of the “crossed scattering channel” of the reaction $\bar{\Pi}_1 + \Pi_2 \rightarrow \bar{\Pi}_1 + \Pi_2$ with squared total energy u . A typical and important example is the case of proton–proton scattering in the s -channel, where M_{12} equals twice the mass $m(=m_1=m_2)$ of the proton, while the corresponding u -channel refers to the proton–anti-proton scattering, whose threshold M'_{12} equals twice the mass μ of the π meson.

In that general case, the analysis of the subsection “‘Off-shell dispersion relations’ as a first step” still applies, so that the function $\hat{H}_{p_2}(\zeta, s)$ is always analytic in a set of the form

$$S_0 = \{(\zeta, s); -a < \zeta < 0, s \in \Delta_\zeta\} \quad [31]$$

Then, the additional information described above in the last subsection allows one to use the following crucial property of analytic completion, which we call

Crossing lemma *If a function $G(\zeta, s)$ is holomorphic in a domain which contains the union of the sets Σ and S_0 (see eqns [30] and [31]), then it admits an analytic continuation in a set of the following form:*

$$\begin{aligned} &\{(\zeta, s); \zeta \in \delta, s \in \Delta_\zeta; \\ &|s - \zeta - m_2^2| = |u - \zeta - m_2^2| > R(\zeta)\} \end{aligned}$$

By applying this property to the function $\hat{H}_{p_2}(\zeta, s)$ and restricting ζ to the mass-shell value m_1^2 which belongs to δ , one obtains the analyticity of the scattering function $\hat{F}_0(s) \doteq \hat{H}_{p_2}(m_1^2, s)$ in a crossing domain of the complex mass shell hyperbola $h^{(c)}[m_1^2]$: the crossing between the two physical regions $h^+[m_1^2]$ ($s \geq M_{12}^2$) and $h^-[m_1^2]$ ($u \geq M_{12}^2$) is ensured by a complex domain of $h^{(c)}[m_1^2]$ whose image in the s -plane is the “cut-neighborhood of infinity” $\{s; s \in \Delta_{m_1^2}, |s - m_1^2 - m_2^2| = |u - m_1^2 - m_2^2| > R(m_1^2)\}$. Note that the relevant boundary values of \hat{F}_0 for obtaining the scattering amplitudes of the two collision processes with respective physical regions $h^+[m_1^2]$ and $h^-[m_1^2]$ have to be taken from the respective sides $\text{Im } s > 0$ and $\text{Im } u = -\text{Im } s > 0$ of the corresponding s - and u -cuts.

It is only for the neutral case, where $M_{12} = M'_{12} = m_1 + m_2$, that a more favorable scenario occurs, as explained earlier: in this case, the interval $\{\zeta \in]-a, 0[\}$ of the set S_0 is replaced by $\{\zeta \in]-a, m_1^2[\}$, so that the whole cut-plane domain $\Delta_{m_1^2}$ is obtained in the result of the previous crossing lemma. The scattering amplitudes of π_0 – π_0 meson scattering and of π meson–proton scattering enjoy this property and, therefore, satisfy genuine dispersion relations in which the scattering function is even (see the second basic example described at the beginning of this article). In the general case of crossing domains obtained above, corresponding Cauchy integral relations have been written and used under the name of “quasi-dispersion-relations.”

Complementary results Some comments can now be added concerning the passage from the purely geometrical results (i.e., analyticity domains) described above to the writing of precise (quasi-) dispersion relations with two subtractions:

Polynomial bounds and dispersion relations with N subtractions The previous methods of analytic completion also allow one to control the bounds at infinity in the relevant complex domains. As it has been noticed after eqn [24], the Fourier–Laplace transforms of the retarded and advanced kernels, and thereby the holomorphic functions $H_{p_2}^\pm(k)$ discussed at the start of this section are bounded at most by a power of a suitable norm of k in their respective tubes \mathcal{T}^\pm . Correspondingly, the holomorphic function $H_{p_2}(k)$ (resp. $H_{p_2}(k_0, k_r)$) admits the same type of bound in its primitive analyticity domain D (resp. D_r). These bounds are a consequence of the tempered distribution character of the structure functions of the fields which is built-in in the Wightman field-theoretical framework. Then it can be checked that in the holomorphy envelope \hat{D}_r of D_r , and thereby in the cut-plane (or crossing) domains obtained in the intersection of \hat{D}_r and of the complex mass shell $h^{(c)}[m_1^2]$, the same type of power bound is still valid: $\hat{F}_0(s)$ is therefore bounded by some power $|s|^{N-1}$ of $|s|$ and thus satisfies a (quasi-)dispersion relation with N subtractions. The same type of argument holds for all the similar cut-domains (or crossing domains) in s obtained for $\hat{F}_t(s)$ for all negative value of t .

It is also worthwhile to mention that a similar remarkable (since not at all predictable) result was also obtained in the Haag, Kastler, and Araki framework of algebraic QFT (Epstein, Glaser, Martin, 1969; see *Scattering in Relativistic Quantum Field Theory: The Analytic Program* for further comments).

In this connection, one can also mention a more recent result. In the Buchholz–Fredenhagen axiomatic approach of charged fields (1982), in which

locality is replaced by the more general notion of “stringlike locality” (see Algebraic Approach to Quantum Field Theory, Axiomatic Quantum Field Theory, and Scattering in Relativistic Quantum Field Theory: Fundamental Concepts and Tools), a proof of forward dispersion relations has again been obtained (Bros, Epstein, 1994).

The extension of the analyticity domains by positivity and the derivation of bounds by unitarity (Martin 1966; see the book by Martin (1969)). The following ingredients have been used:

1. Positivity conditions on the absorptive part of $F(s, t)$, which are expressed by the infinite set of inequalities $(d/dt)^n \text{Im} F(s, t)|_{t=0} \geq 0$ (for all integers n),
2. The existence of a two-dimensional complex neighborhood of some point $(s = s_0, t = 0)$ in the analyticity domain resulting from QFT.

The following results have then been obtained:

- (a) It is justified to differentiate the forward (subtracted) dispersion relations with respect to t at any order.
- (b) $\hat{F}(s, t)$ can be analytically continued in a fixed circle $|t| < t_{\max}$ for all values of s . The latter implies the extension of dispersion relations in s to positive (and complex) values of t .
- (c) In a last step, the use of unitarity conditions for the “partial waves” $f_\ell(s)$ of $F(s, t)$ (see Scattering in Relativistic Quantum Field Theory: The Analytic Program) allows one to obtain

Froissart-type bounds on the scattering amplitudes and thereby to justify the writing of (quasi-)dispersion relations with at most two subtractions for all the admissible values of t .

See also: Algebraic Approach to Quantum Field Theory; Axiomatic Quantum Field Theory; Perturbation Theory and its Techniques; Scattering in Relativistic Quantum Field Theory: The Analytic Program; Scattering, Asymptotic Completeness and Bound States; Scattering in Relativistic Quantum Field Theory: Fundamental Concepts and Tools.

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Dissipative Dynamical Systems of Infinite Dimension

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Introduction

A dynamical system (DS) is a system which evolves with respect to the time. To be more precise, a DS $(S(t), \Phi)$ is determined by a phase space Φ which consists of all possible values of the parameters describing the state of the system and an evolution map $S(t): \Phi \rightarrow \Phi$ that allows one to find the state of the system at time $t > 0$ if the initial state at $t = 0$ is known. Very often, in mechanics and physics, the evolution of the system is governed by systems of

differential equations. If the system is described by ordinary differential equations (ODEs),

$$\frac{d}{dt} y(t) = F(t, y(t)), \quad y(0) = y_0, \\ y(t) := (y_1(t), \dots, y_N(t)) \quad [1]$$

for some nonlinear function $F: \mathbb{R}_+ \times \mathbb{R}^N \rightarrow \mathbb{R}^N$, we have a so-called finite-dimensional DS. In that case, the phase space Φ is some (invariant) subset of \mathbb{R}^N and the evolution operator $S(t)$ is defined by

$$S(t)y_0 := y(t), \quad y(t) \text{ solves } [1] \quad [2]$$

We also recall that, in the case where eqn [1] is autonomous (i.e., does not depend explicitly on the time), the evolution operators $S(t)$ generate a semigroup on the phase space Φ , that is,

$$S(t_1 + t_2) = S(t_1) \circ S(t_2), \quad t_1, t_2 \in \mathbb{R}_+ \quad [3]$$

Now, in the case of a distributed system whose initial state is described by functions $u_0 = u_0(x)$ depending on the spatial variable x , the evolution is usually governed by partial differential equations (PDEs) and the corresponding phase space Φ is some infinite-dimensional function space (e.g., $\Phi := L^2(\Omega)$ or $\Phi := L^\infty(\Omega)$ for some domain $\Omega \subset \mathbb{R}^N$.) Such DSs are usually called infinite dimensional.

The qualitative study of DSs of finite dimensions goes back to the beginning of the twentieth century, with the pioneering works of Poincaré on the N -body problem (one should also acknowledge the contributions of Lyapunov on the stability and of Birkhoff on the minimal sets and the ergodic theorem). One of the most surprising and significant facts discovered at the very beginning of the theory is that even relatively simple equations can generate very complicated chaotic behaviors. Moreover, these types of systems are extremely sensitive to initial conditions (the trajectories with close but different initial data diverge exponentially). Thus, in spite of the deterministic nature of the system (we recall that it is generated by a system of ODEs, for which we usually have the unique solvability theorem), its temporal evolution is unpredictable on timescales larger than some critical time T_0 (which depends obviously on the error of approximation and on the rate of divergence of close trajectories) and can show typical stochastic behaviors. To the best of our knowledge, one of the first ODEs for which such types of behaviors were established is the physical pendulum parametrically perturbed by time-periodic external forces,

$$y''(t) + \sin(y(t))(1 + \varepsilon \sin(\omega t)) = 0 \quad [4]$$

where ω and $\varepsilon > 0$ are physical parameters. We also mention the more recent (and more relevant for our topic) famous example of the Lorenz system which is defined by the following system of ODEs in \mathbb{R}^3 :

$$\begin{cases} x' = \sigma(y - x) \\ y' = -xy + rx - y \\ z' = xy - bz \end{cases} \quad [5]$$

where σ, r , and b are some parameters. These equations are obtained by truncation of the Navier–Stokes equations and give an approximate description of a horizontal fluid layer heated from below. The warmer fluid formed at the bottom tends to rise, creating convection currents. This is similar to what happens in the Earth's atmosphere. For a sufficiently intense heating, the time evolution has a sensitive dependence on the initial conditions, thus representing a very irregular and chaotic

convection. This fact was used by Lorenz to justify the so-called “butterfly effect,” a metaphor for the imprecision of weather forecast.

The theory of DSs in finite dimensions had been extensively developed during the twentieth century, due to the efforts of many famous mathematicians (such as Anosov, Arnold, LaSalle, Sinai, Smale, etc.) and, nowadays, much is known on the chaotic behaviors in such systems, at least in low dimensions. In particular, it is known that, very often, the trajectories of a chaotic system are localized, up to a transient process, in some subset of the phase space having a very complicated fractal geometric structure (e.g., locally homeomorphic to the Cartesian product of \mathbb{R}^m and some Cantor set) which, thus, accumulates the nontrivial dynamics of the system (the so-called strange attractor). The chaotic dynamics on such sets are usually described by symbolic dynamics generated by Bernoulli shifts on the space of sequences. We also note that, nowadays, a mathematician has a large amount of different concepts and methods for the extensive study of concrete chaotic DSs in finite dimensions. In particular, we mention here different types of bifurcation theories (including the KAM theory and the homoclinic bifurcation theory with related Shilnikov chaos), the theory of hyperbolic sets, stochastic description of deterministic processes, Lyapunov exponents and entropy theory, dynamical analysis of time series, etc.

We now turn to infinite-dimensional DSs generated by PDEs. A first important difficulty which arises here is related to the fact that the analytic structure of a PDE is essentially more complicated than that of an ODE and, in particular, we do not have in general the unique solvability theorem as for ODEs, so that even finding the proper phase space and the rigorous construction of the associated DS can be a highly nontrivial problem. In order to indicate the level of difficulties arising here, it suffices to recall that, for the three-dimensional Navier–Stokes system (which is one of the most important equations of mathematical physics), the required associated DS has not been constructed yet. Nevertheless, there exists a large number of equations for which the problem of the global existence and uniqueness of a solution has been solved. Thus, the question of extending the highly developed finite-dimensional DS theory to infinite dimensions arises naturally.

One of the first and most significant results in that direction was the development of the theory of integrable Hamiltonian systems in infinite dimensions and the explicit resolution (by inverse-scattering methods) of several important conservative equations

of mathematical physics (such as the Korteweg-de Vries (and the generalized Kadomtsev-Petviashvili hierarchy), the sine-Gordon, and the nonlinear Schrödinger equations). Nevertheless, it is worth noting that integrability is a very rare phenomenon, even among ODEs, and this theory is clearly insufficient to understand the dynamics arising in PDEs. In particular, there exist many important equations which are essentially out of reach of this theory.

One of the most important classes of such equations consists of the so-called dissipative PDEs which are the main subject of our study. As hinted by this denomination, these systems exhibit some energy dissipation process (in contrast to conservative systems for which the energy is preserved) and, of course, in order to have nontrivial dynamics, these models should also account for the energy income. Roughly speaking, the complicated chaotic behaviors in such systems usually arise from the interaction of the following mechanisms:

1. energy dissipation in the higher part of the Fourier spectrum;
2. external energy income in its lower part;
3. energy flux from lower to higher Fourier modes provided by the nonlinear terms of the equation.

We chose not to give a rigorous definition of a dissipative system here (although the concepts of energy dissipation and related dissipative systems are more or less obvious from the physical point of view, they seem too general to have an adequate mathematical definition). Instead, we only indicate several basic classes of equations of mathematical physics which usually exhibit the above behaviors.

The first example is, of course, the Navier-Stokes system, which describes the motion of a viscous incompressible fluid in a bounded domain Ω (we will only consider here the two-dimensional case $\Omega \subset \mathbb{R}^2$, since the adequate formulation in three dimensions is still an open problem):

$$\begin{cases} \partial_t u - (u, \nabla_x)u = \nu \Delta_x u + \nabla_x p + g(x) \\ \operatorname{div} u = 0, u|_{t=0} = u_0, u|_{\partial\Omega} = 0 \end{cases} \quad [6]$$

Here, $u(t, x) = (u_1(t, x), u_2(t, x))$ is the unknown velocity vector, $p = p(t, x)$ is the unknown pressure, Δ_x is the Laplacian with respect to x , $\nu > 0$ and g are given kinematic viscosity and external forces, respectively, and $(u, \nabla_x)u$ is the inertial term ($[(u, \nabla_x)u]_i = \sum_{j=1}^2 u_j \partial_{x_j} u_i$, $i = 1, 2$). The unique global solvability of [6] has been proved by Ladyzhenskaya. Thus, this equation generates an infinite-dimensional DS in the phase space Φ of divergence-free square-integrable vector fields.

The second example is the damped nonlinear wave equation in $\Omega \subset \mathbb{R}^n$:

$$\begin{aligned} \partial_t^2 u + \gamma \partial_t u - \Delta_x u + f(u) &= 0 \\ u|_{\partial\Omega} &= 0, \quad u|_{t=0} = u_0, \quad \partial_t u|_{t=0} = u'_0 \end{aligned} \quad [7]$$

which models, for example, the dynamics of a Josephson junction driven by a current source (sine-Gordon equation). It is known that, under natural sign and growth assumptions on the nonlinear interaction function f , this equation generates a DS in the energy phase space E of pairs of functions $(u, \partial_t u)$ such that $\partial_t u$ and $\nabla_x u$ are square integrable.

The last class of equations that we will consider here consists of reaction-diffusion systems in a domain $\Omega \subset \mathbb{R}^n$:

$$\partial_t u = a \Delta_x u - f(u), \quad u|_{t=0} = u_0 \quad [8]$$

(endowed with Dirichlet ($u|_{\partial\Omega} = 0$) or Neumann ($\partial_n u|_{\partial\Omega} = 0$) boundary conditions), which describes some chemical reaction in Ω . Here, $u = (u^1, \dots, u^N)$ is an unknown vector-valued function which describes the concentrations of the reactants, $f(u)$ is a given interaction function, and a is a diffusion matrix. It is known that, under natural assumptions on f and a , these equations also generate an infinite-dimensional DS, for example, in the phase space $\Phi := [L^\infty(\Omega)]^N$.

We emphasize once more that the phase spaces Φ in all these examples are appropriate infinite-dimensional function spaces. Nevertheless, it was observed in experiments that, up to a transient process, the trajectories of the DS considered are localized inside a "very thin" invariant subset of the phase space having a complicated geometric structure which, thus, accumulates all the nontrivial dynamics of the system. It was conjectured a little later that these invariant sets are, in some proper sense, finite dimensional and that the dynamics restricted to these sets can be effectively described by a finite number of parameters. Thus (when this conjecture is true), in spite of the infinite-dimensional initial phase space, the effective dynamics (reduced to this invariant set) is finite dimensional and can be studied by using the algorithms and concepts of the classical finite-dimensional DS theory. In particular, this means that the infinite dimensionality plays here only the role of (possibly essential) technical difficulties, which cannot, however, produce any new dynamical phenomena which are not observed in the finite-dimensional theory.

The above finite-dimensional reduction principle of dissipative PDEs in bounded domains has been given solid mathematical grounds (based on the concept of the so-called global attractor) over the

last three decades, starting from the pioneering papers of Ladyzhenskaya. This theory is considered in more detail here.

The finite-dimensional reduction theory has some limitations. Of course, the first and most obvious restriction of this principle is the effective dimension of the reduced finite-dimensional DS. Indeed, it is known that, typically, this dimension grows at least linearly with respect to the volume $\text{vol}(\Omega)$ of the spatial domain Ω of the DS considered (and the growth of the size of Ω is the same (up to a rescaling) as the decay of the viscosity coefficient ν or the diffusion matrix a , see eqns [6]–[8]). So, for sufficiently large domains Ω , the reduced DS can be too large for reasonable investigations.

The next, less obvious, but much more essential, restriction is the growing spatial complexity of the DS. Indeed, as shown by Babin–Buinimovich, the spatial complexity of the system (e.g., the number of topologically different equilibria) grows exponentially with respect to $\text{vol}(\Omega)$. Thus, even in the case of relatively small dimensions, the reduced system can be out of reasonable investigations, due to its extremely complicated structure.

Therefore, the approach based on the finite-dimensional reduction does not look so attractive for large domains. It seems, instead, more natural, at least from the physical point of view, to replace large bounded domains by their limit unbounded ones (e.g., $\Omega = \mathbb{R}^n$ or cylindrical domains). Of course, this approach requires a systematic study of dissipative DSs associated with PDEs in unbounded domains.

The dynamical study of PDEs in unbounded domains started from the pioneering paper of Kolmogorov–Petrovskij–Piskunov, in which the traveling wave solutions of reaction–diffusion equations in a strip were constructed and the convergence of the trajectories (for specific initial data) to this traveling wave solutions were established. Starting from this, many results on the dynamics of PDE in unbounded domains have been obtained. However, for a long period, the general features of such dynamics remained completely unclear. The main problems arising here are:

1. the essential infinite dimensionality of the DS considered (absence of any finite-dimensional reduction), which leads to essentially new dynamical effects that are not observed in finite-dimensional theories;
2. the additional spatial “unbounded” directions lead to the so-called spatial chaos and the interaction between spatial and temporal chaotic modes generates the spatio-temporal chaos, which also has no analog in finite dimensions.

Nevertheless, several ideas are mentioned in the following which (from authors’ point of view) were the most important for the development of these topics. The first one is the pioneering paper of Kirchgässner, in which dynamical methods were applied to the study of the spatial structure of solutions of elliptic equations in cylinders (which can be considered as equilibria equations for evolution PDEs in unbounded cylindrical domains). The second is the Sinai–Buinimovich model of spacetime chaos in discrete lattice DSs. Finally, the third is the adaptation of the concept of a global attractor to unbounded domains by Abergel and Babin–Vishik.

We note that the situation on the understanding of the general features of the dynamics in unbounded domains, however, seems to have changed in the last several years, due to the works of Collet–Eckmann and Zelik. This is the reason why a section of this review is devoted to a more detailed discussion on this topic.

Other important questions are the object of current studies and we only briefly mention some of them. We mention for instance, the study of attractors for nonautonomous systems (i.e., systems in which the time appears explicitly). This situation is much more delicate and is not completely understood; notions of attractors for such systems have been proposed by Chepyzhov–Vishik, Haraux and Kloeden–Schmalfuss. We also mention that theories of (global) attractors for non-well-posed problems have been proposed by Babin–Vishik, Ball, Chepyzhov–Vishik, Melnik–Valero, and Sell.

Global Attractors and Finite-Dimensional Reduction

Global Attractors: The Abstract Setting

As already mentioned, one of the main concepts of the modern theory of DSs in infinite dimensions is that of the global attractor. We give below its definition for an abstract semigroup $S(t)$ acting on a metric space Φ , although, without loss of generality, the reader may think that $(S(t), \Phi)$ is just a DS associated with one of the PDEs ([6]–[8]) described in the introduction.

To this end, we first recall that a subset K of the phase space Φ is an attracting set of the semigroup $S(t)$ if it attracts the images of all the bounded subsets of Φ , that is, for every bounded set B and every $\varepsilon > 0$, there exists a time T (depending in general on B and ε) such that the image $S(t)B$ belongs to the

ε -neighborhood of K if $t \geq T$. This property can be rewritten in the equivalent form

$$\lim_{t \rightarrow \infty} \text{dist}_H(S(t)B, K) = 0 \quad [9]$$

where $\text{dist}_H(X, Y) := \sup_{x \in X} \inf_{y \in Y} d(x, y)$ is the non-symmetric Hausdorff distance between subsets of Φ .

The following definition of a global attractor is due to Babin–Vishik.

Definition 1 A set $\mathcal{A} \subset \Phi$ is a global attractor for the semigroup $S(t)$ if

- (i) \mathcal{A} is compact in Φ ;
- (ii) \mathcal{A} is strictly invariant: $S(t)\mathcal{A} = \mathcal{A}$, for all $t \geq 0$;
- (iii) \mathcal{A} is an attracting set for the semigroup $S(t)$.

Thus, the second and third properties guarantee that a global attractor, if it exists, is unique and that the DS reduced to the attractor contains all the nontrivial dynamics of the initial system. Furthermore, the first property indicates that the reduced phase space \mathcal{A} is indeed “thinner” than the initial phase space Φ (we recall that, in infinite dimensions, a compact set cannot contain, e.g., balls and should thus be nowhere dense).

In most applications, one can use the following attractor’s existence theorem.

Theorem 1 Let a DS $(S(t), \Phi)$ possess a compact attracting set and the operators $S(t): \Phi \rightarrow \Phi$ be continuous for every fixed t . Then, this system possesses the global attractor \mathcal{A} which is generated by all the trajectories of $S(t)$ which are defined for all $t \in \mathbb{R}$ and are globally bounded.

The strategy for applying this theorem to concrete equations of mathematical physics is the following. In a first step, one verifies a so-called dissipative estimate which has usually the form

$$\|S(t)u_0\|_\Phi \leq Q(\|u_0\|_\Phi) e^{-\alpha t} + C_*, \quad u_0 \in \Phi \quad [10]$$

where $\|\cdot\|_\Phi$ is a norm in the function space Φ and the positive constants α and C_* and the monotonic function Q are independent of t and $u_0 \in \Phi$ (usually, this estimate follows from energy estimates and is sometimes even used in order to “define” a dissipative system). This estimate obviously gives the existence of an attracting set for $S(t)$ (e.g., the ball of radius $2C_*$ in Φ), which is, however, noncompact in Φ . In order to overcome this problem, one usually derives, in a second step, a smoothing property for the solutions, which can be formulated as follows:

$$\|S(1)u_0\|_{\Phi_1} \leq Q_1(\|u_0\|_\Phi), \quad u_0 \in \Phi \quad [11]$$

where Φ_1 is another function space which is compactly embedded into Φ . In applications, Φ is

usually the space $L^2(\Omega)$ of square integrable functions, Φ_1 is the Sobolev space $H^1(\Omega)$ of the functions u such that u and $\nabla_x u$ belong to $L^2(\Omega)$ and estimate [11] is a classical smoothing property for solutions of parabolic equations (for hyperbolic equations, a slightly more complicated asymptotic smoothing property should be used instead of [11]).

Since the continuity of the operators $S(t)$ usually arises no difficulty (if the uniqueness is proven), then the above scheme gives indeed the existence of the global attractor for most of the PDEs of mathematical physics in bounded domains.

Dimension of the Global Attractor

In this subsection, we start by discussing one of the basic questions of the theory: in which sense is the dynamics on the global attractor finite dimensional? As already mentioned, the global attractor is usually not a manifold, but has a rather complicated geometric structure. So, it is natural to use the definitions of dimensions adopted for the study of fractal sets here. We restrict ourselves to the so-called fractal (or box-counting, entropy) dimension, although other dimensions (e.g., Hausdorff, Lyapunov, etc.) are also used in the theory of attractors.

In order to define the fractal dimension, we first recall the concept of Kolmogorov’s ε -entropy, which comes from the information theory and plays a fundamental role in the theory of DSs in unbounded domains considered in the next section.

Definition 2 Let \mathcal{A} be a compact subset of a metric space Φ . For every $\varepsilon > 0$, we define $N_\varepsilon(K)$ as the minimal number of ε -balls which are necessary to cover \mathcal{A} . Then, Kolmogorov’s ε -entropy $\mathcal{H}_\varepsilon(\mathcal{A}) = \mathcal{H}_\varepsilon(\mathcal{A}, \Phi)$ of \mathcal{A} is the digital logarithm of this number, $\mathcal{H}_\varepsilon(\mathcal{A}) := \log_2 N_\varepsilon(\mathcal{A})$. We recall that $\mathcal{H}_\varepsilon(\mathcal{A})$ is finite for every $\varepsilon > 0$, due to the Hausdorff criterium. The fractal dimension $d_f(\mathcal{A}) \in [0, \infty]$ of \mathcal{A} is then defined by

$$d_f(\mathcal{A}) := \limsup_{\varepsilon \rightarrow 0} \mathcal{H}_\varepsilon(\mathcal{A}) / \log_2 1/\varepsilon \quad [12]$$

We also recall that, although this dimension coincides with the usual dimension of the manifold for Lipschitz manifolds, it can be noninteger for more complicated sets. For instance, the fractal dimension of the standard ternary Cantor set in $[0, 1]$ is $\ln 2 / \ln 3$.

The so-called Mané theorem (which can be considered as a generalization of the classical Yitni embedding theorem for fractal sets) plays an important role in the finite-dimensional reduction theory.

Theorem 2 *Let Φ be a Banach space and \mathcal{A} be a compact set such that $d_f(\mathcal{A}) < N$ for some $N \in \mathbb{N}$. Then, for “almost all” $(2N+1)$ -dimensional planes L in Φ , the corresponding projector $\Pi_L: \Phi \rightarrow L$ restricted to the set \mathcal{A} is a Hölder continuous homeomorphism.*

Thus, if the finite fractal dimensionality of the attractor is established, then, fixing a hyperplane L satisfying the assumptions of the Mané theorem and projecting the attractor \mathcal{A} and the DS $S(t)$ restricted to \mathcal{A} onto this hyperplane ($\bar{\mathcal{A}} := \Pi_L \mathcal{A}$ and $\bar{S}(t) := \Pi_L \circ S(t) \circ \Pi_L^{-1}$), we obtain, indeed, a reduced DS $(\bar{S}(t), \bar{\mathcal{A}})$ which is defined on a finite-dimensional set $\bar{\mathcal{A}} \subset L \sim \mathbb{R}^{2N+1}$. Moreover, this DS will be Hölder continuous with respect to the initial data.

Estimates on the Fractal Dimension

Obviously, good estimates on the dimension of the attractors in terms of the physical parameters are crucial for the finite-dimensional reduction described above, and (consequently) there exists a highly developed machinery for obtaining such estimates. The best-known upper estimates are usually obtained by the so-called volume contraction method, which is based on the study of the evolution of infinitesimal k -dimensional volumes in the neighborhood of the attractor (and, if the DS considered contracts the k -dimensional volumes, then the fractal dimension of the attractor is less than k). Lower bounds on the dimension are usually based on the observation that the global attractor always contains the unstable manifolds of the (hyperbolic) equilibria. Thus, the instability index of a properly constructed equilibrium gives a lower bound on the dimension of the attractor.

In the following, several estimates for the classes of equations given in the introduction are formulated, beginning with the most-studied case of the reaction–diffusion system [8]. For this system, sharp upper and lower bounds are known, namely

$$C_1 \text{vol}(\Omega) \leq d_f(\mathcal{A}) \leq C_2 \text{vol}(\Omega) \quad [13]$$

where the constants C_1 and C_2 depend on a and f (and, possibly, on the shape of Ω), but are independent of its size. The same types of estimates also hold for the hyperbolic equation [7]. Concerning the Navier–Stokes system [6] in general two-dimensional domains Ω , the asymptotics of the fractal dimension as $\nu \rightarrow 0$ is not known. The best-known upper bound has the form $d_f(\mathcal{A}) \leq C\nu^{-2}$ and was obtained by Foias–Temam by using the so-called Lieb–Thirring

inequalities. Nevertheless, for periodic boundary conditions, Constantin–Foias–Temam and Liu obtained upper and lower bounds of the same order (up to a logarithmic correction):

$$C_1 \nu^{-4/3} \leq d_f(\mathcal{A}) \leq C_2 \nu^{-4/3} (1 + \ln(\nu^{-1}))^{1/3} \quad [14]$$

Global Lyapunov Functions and the Structure of Global Attractors

Although the global attractor has usually a very complicated geometric structure, there exists one exceptional class of DS for which the global attractor has a relatively simple structure which is completely understood, namely the DS having a global Lyapunov function. We recall that a continuous function $\mathcal{L}: \Phi \rightarrow \mathbb{R}$ is a global Lyapunov function if

1. \mathcal{L} is nonincreasing along the trajectories, that is, $\mathcal{L}(S(t)u_0) \leq \mathcal{L}(u_0)$, for all $t \geq 0$;
2. \mathcal{L} is strictly decreasing along all nonequilibrium solutions, that is, $\mathcal{L}(S(t)u_0) = \mathcal{L}(u_0)$ for some $t > 0$ and u_0 implies that u_0 is an equilibrium of $S(t)$.

For instance, in the scalar case $N=1$, the reaction–diffusion equations [8] possess the global Lyapunov function $\mathcal{L}(u_0) := \int_{\Omega} [a|\nabla_x u_0(x)|^2 + F(u_0(x))] dx$, where $F(v) := \int_0^v f(u) du$. Indeed, multiplying eqn [8] by $\partial_t u$ and integrating over Ω , we have

$$\frac{d}{dt} \mathcal{L}(u(t)) = -2 \|\partial_t u(t)\|_{L^2(\Omega)}^2 \leq 0 \quad [15]$$

Analogously, in the scalar case $N=1$, multiplying the hyperbolic equation [7] by $\partial_t u(t)$ and integrating over Ω , we obtain the standard global Lyapunov function for this equation.

It is well known that, if a DS possesses a global Lyapunov function, then, at least under the generic assumption that the set \mathcal{R} of equilibria is finite, every trajectory $u(t)$ stabilizes to one of these equilibria as $t \rightarrow +\infty$. Moreover, every complete bounded trajectory $u(t)$, $t \in \mathbb{R}$, belonging to the attractor is a heteroclinic orbit joining two equilibria. Thus, the global attractor \mathcal{A} can be described as follows:

$$\mathcal{A} = \bigcup_{u_0 \in \mathcal{R}} \mathcal{M}^+(u_0) \quad [16]$$

where $\mathcal{M}^+(u_0)$ is the so-called unstable set of the equilibrium u_0 (which is generated by all heteroclinic orbits of the DS which start from the given equilibrium $u_0 \in \mathcal{A}$). It is also known that, if the equilibrium u_0 is hyperbolic (generic assumption), then the set $\mathcal{M}^+(u_0)$ is a κ -dimensional submanifold of Φ , where κ is the instability index of u_0 . Thus, under the generic hyperbolicity assumption on the equilibria, the

attractor \mathcal{A} of a DS having a global Lyapunov function is a finite union of smooth finite-dimensional submanifolds of the phase space Φ . These attractors are called regular (following Babin–Vishik).

It is also worth emphasizing that, in contrast to general global attractors, regular attractors are robust under perturbations. Moreover, in some cases, it is also possible to verify the so-called transversality conditions (for the intersection of stable and unstable manifolds of the equilibria) and, thus, verify that the DS considered is a Morse–Smale system. In particular, this means that the dynamics restricted to the regular attractor \mathcal{A} is also preserved (up to homeomorphisms) under perturbations.

A disadvantage of the approach of using a regular attractor is the fact that, except for scalar parabolic equations in one space dimension, it is usually extremely difficult to verify the “generic” hyperbolicity and transversality assumptions for concrete values of the physical parameters and the associated hyperbolicity constants, as a rule, cannot be expressed in terms of these parameters.

Inertial Manifolds

It should be noted that the scheme for the finite-dimensional reduction described above has essential drawbacks. Indeed, the reduced system $(\tilde{S}(t), \tilde{\mathcal{A}})$ is only Hölder continuous and, consequently, cannot be realized as a DS generated by a system of ODEs (and reasonable conditions on the attractor \mathcal{A} which guarantee the Lipschitz continuity of the Mané projections are not known). On the other hand, the complicated geometric structure of the attractor \mathcal{A} (or $\tilde{\mathcal{A}}$) makes the use of this finite-dimensional reduction in computations hazardous (in fact, only the heuristic information on the number of unknowns which are necessary to capture all the dynamical effects in approximations can be extracted).

In order to overcome these problems, the concept of an inertial manifold (which allows one to embed the global attractor into a smooth manifold) has been suggested by Foias–Sell–Temam. To be more precise, a Lipschitz finite-dimensional manifold $\mathbb{M} \subset \Phi$ is an inertial manifold for the DS $(S(t), \Phi)$ if

1. \mathbb{M} is semiinvariant, that is, $S(t)\mathbb{M} \subset \mathbb{M}$, for all $t \geq 0$;
2. \mathbb{M} satisfies the following asymptotic completeness property: for every $u_0 \in \Phi$, there exists $v_0 \in \mathbb{M}$ such that

$$\|S(t)u_0 - S(t)v_0\|_{\Phi} \leq Q(\|u_0\|_{\Phi})e^{-\alpha t} \quad [17]$$

where the positive constant α and the monotonic function Q are independent of u_0 .

We can see that an inertial manifold, if it exists, confirms in a perfect way the heuristic conjecture on the finite dimensionality formulated in the introduction. Indeed, the dynamics of $S(t)$ restricted to an inertial manifold can be, obviously, described by a system of ODEs (which is called the inertial form of the initial PDE). On the other hand, the asymptotic completeness gives (in a very strong form) the equivalence of the initial DS $(S(t), \Phi)$ with its inertial form $(S(t), \mathbb{M})$. Moreover, in turbulence, the existence of an inertial manifold would yield an exact interaction law between the small and large structures of the flow.

Unfortunately, all the known constructions of inertial manifolds are based on a very restrictive condition, the so-called spectral gap condition, which requires arbitrarily large gaps in the spectrum of the linearization of the initial PDE and which can usually be verified only in one space dimension. So, the existence of an inertial manifold is still an open problem for many important equations of mathematical physics (including in particular the two-dimensional Navier–Stokes equations; some nonexistence results have also been proven by Mallet–Paret).

Exponential Attractors

We first recall that Definition 1 of a global attractor only guarantees that the images $S(t)B$ of all the bounded subsets converge to the attractor, without saying anything on the rate of convergence (in contrast to inertial manifolds, for which this rate of convergence can be controlled). Furthermore, as elementary examples show, this convergence can be arbitrarily slow, so that, until now, we have no effective way for estimating this rate of convergence in terms of the physical parameters of the system (an exception is given by the regular attractors described earlier for which the rate of convergence can be estimated in terms of the hyperbolicity constants of the equilibria. However, even in this situation, it is usually very difficult to estimate these constants for concrete equations). Furthermore, there exist many physically relevant systems (e.g., the so-called slightly dissipative gradient systems) which have trivial global attractors, but very rich and physically relevant transient dynamics which are automatically forgotten under the global-attractor approach. Another important problem is the robustness of the global attractor under perturbations. In fact, global attractors are usually only upper semicontinuous under

perturbations (which means that they cannot explode) and the lower semicontinuity (which means that they cannot also implode) is much more delicate to prove and requires some hyperbolicity assumptions (which are usually impossible to verify for concrete equations).

In order to overcome these difficulties, Eden–Foias–Nicolaenko–Temam have introduced an intermediate object (between inertial manifolds and global attractors), namely an exponential attractor (also called an inertial set).

Definition 3 A compact set $\mathcal{M} \subset \Phi$ is an exponential attractor for the DS $(S(t), \Phi)$ if

- (i) \mathcal{M} has finite fractal dimension: $d_f(\mathcal{M}) < \infty$;
- (ii) \mathcal{M} is semi-invariant: $S(t)\mathcal{M} \subset \mathcal{M}$, for all $t \geq 0$;
- (iii) \mathcal{M} attracts exponentially the images of all the bounded sets $B \subset \Phi$:

$$\text{dist}_H(S(t)B, \mathcal{M}) \leq Q(\|B\|_\Phi)e^{-\alpha t} \quad [18]$$

where the positive constant α and the monotonic function Q are independent of B .

Thus, on the one hand, an exponential attractor remains finite dimensional (like the global attractor) and, on the other hand, estimate [18] allows one to control the rate of attraction (like an inertial manifold). We note, however, that the relaxation of strict invariance to semi-invariance allows this object to be nonunique. So, we have here the problem of the “best choice” of the exponential attractor. We also mention that an exponential attractor, if it exists, always contains the global attractor.

Although the initial construction of exponential attractors is based on the so-called squeezing property (and requires Zorn’s lemma), we formulate below a simpler construction, due to Efendiev–Miranville–Zelik, which is similar to the method proposed by Ladyzhenskaya to verify the finite dimensionality of global attractors. This is done for discrete times and for a DS generated by iterations of some map $S: \Phi \rightarrow \Phi$, since the passage from discrete to continuous times usually arises no difficulty (without loss of generality, the reader may think that $S = S(1)$ and $(S(t), \Phi)$ is one of the DS mentioned in the introduction).

Theorem 3 Let the phase space Φ_0 be a closed bounded subset of some Banach space H and let H_1 be another Banach space compactly embedded into H . Assume also that the map $S: \Phi_0 \rightarrow \Phi_0$ satisfies the following “smoothing” property:

$$\|Su_1 - Su_2\|_{H_1} \leq K\|u_1 - u_2\|_H, \quad u_1, u_2 \in \Phi_0 \quad [19]$$

for some constant K independent of u_i . Then, the DS (S, Φ_0) possesses an exponential attractor.

In applications, Φ_0 is usually a bounded absorbing/attracting set whose existence is guaranteed by the dissipative estimate [10], $H := L^2(\Omega)$ and $H_1 := H^1(\Omega)$. Furthermore, estimate [19] simply follows from the classical parabolic smoothing property, but now applied to the equation of variations (as in [11], hyperbolic equations require a slightly more complicated analogue of [19]). These simple arguments show that exponential attractors are as general as global attractors and, to the best of our knowledge, exponential attractors exist indeed for all the equations of mathematical physics for which the finite dimensionality of the global attractor can be established. Moreover, since $\mathcal{A} \subset \mathcal{M}$, this scheme can also be used to prove the finite dimensionality of global attractors.

It is finally worth emphasizing that the control on the rate of convergence provided by [18] makes exponential attractors much more robust than global attractors. In particular, they are upper and lower semicontinuous under perturbations (of course, up to the “best choice,” since they are not unique), as shown by Efendiev–Miranville–Zelik.

Essentially Infinite-Dimensional Dynamical Systems – The Case of Unbounded Domains

As already mentioned in the introduction, the theory of dissipative DS in unbounded domains is developing only now and the results given here are not as complete as for bounded domains. Nevertheless, we indicate below several of the most interesting (from our point of view) results concerning the general description of the dynamics generated by such problems by considering a system of reaction–diffusion equations [8] in \mathbb{R}^n with phase space $\Phi = L^\infty(\mathbb{R}^n)$ as a model example (although all the results formulated below are general and depend weakly on the choice of equation).

Generalization of the Global Attractor and Kolmogorov’s ε -Entropy

We first note that Definition 1 of a global attractor is too strong for equations in unbounded domains. Indeed, as seen earlier, the compactness of the attractor is usually based on the compactness of the embedding $H^1(\Omega) \subset L^2(\Omega)$, which does not hold in unbounded domains. Furthermore, an attractor, in the sense of Definition 1, does not exist for most of the interesting examples of eqns [8] in \mathbb{R}^n .

It is natural to use instead the concept of the so-called locally compact global attractor which is well adapted to unbounded domains. This attractor \mathcal{A} is only bounded in the phase space $\Phi = L^\infty(\mathbb{R}^n)$, but its restrictions $\mathcal{A}|_\Omega$ to all bounded domains Ω are compact in $L^\infty(\Omega)$. Moreover, the attraction property should also be understood in the sense of a local topology in $L^\infty(\mathbb{R}^n)$. It is known that this generalized global attractor \mathcal{A} exists indeed for problem [8] in \mathbb{R}^n (of course, under some “natural” assumptions on the nonlinearity f and the diffusion matrix a). As for bounded domains, its existence is based on the dissipative estimate [10], the smoothing property [11], and the compactness of the embedding $H_{\text{loc}}^1(\mathbb{R}^n) \subset L_{\text{loc}}^2(\mathbb{R}^n)$ (we need to use the local topology only to have this compactness).

The next natural question that arises here is how to control the “size” of the attractor \mathcal{A} if its fractal dimension is infinite (which is usually the case in unbounded domains). One of the most natural ways to handle this problem (which was first suggested by Chepyzhov–Vishik in the different context of uniform attractors associated with nonautonomous equations in bounded domains and appears as extremely fruitful for the theory of dissipative PDE in unbounded domains) is to study the asymptotics of Kolmogorov’s ε -entropy of the attractor. Actually, since the attractor \mathcal{A} is compact only in a local topology, it is natural to study the entropy of its restrictions, say, to balls $B_{x_0}^R$ of \mathbb{R}^n of radius R centered at x_0 with respect to the three parameters R, x_0 , and ε . A more or less complete answer to this question is given by the following estimate:

$$\mathcal{H}_\varepsilon(\mathcal{A}|_{B_{x_0}^R}) \leq C(R + \log_2 1/\varepsilon)^n \log_2 1/\varepsilon \quad [20]$$

where the constant C is independent of $\varepsilon \leq 1$, R , and x_0 . Moreover, it can be shown that this estimate is sharp for all R and ε under the very weak additional assumption that eqn [8] possesses at least one exponentially unstable spatially homogeneous equilibrium.

Thus, formula [20] (whose proof is also based on a smoothing property for the equation of variations) can be interpreted as a natural generalization of the heuristic principle of finite dimensionality of global attractors to unbounded domains. It is also worth recalling that the entropy of the embedding of a ball \mathcal{B}_k of the space $C^k(B_{x_0}^R)$ into $C(B_{x_0}^R)$ has the asymptotic $\mathcal{H}_\varepsilon(\mathcal{B}) \sim C_R(1/\varepsilon)^{n/k}$, which is essentially worse than [20]. So, [20] is not based on the smoothness of the attractor \mathcal{A} and, therefore, reflects deeper properties of the equation.

Spatial Dynamics and Spatial Chaos

The next main difference with bounded domains is the existence of unbounded spatial directions which can generate the so-called spatial chaos (in addition to the “usual” temporal chaos arising under the evolution). In order to describe this phenomenon, it is natural to consider the group $\{T_b, b \in \mathbb{R}^n\}$ of spatial translations acting on the attractor \mathcal{A} :

$$(T_b u_0)(x) := u_0(x + b), \quad T_b : \mathcal{A} \rightarrow \mathcal{A} \quad [21]$$

as a DS (with multidimensional “times” if $n > 1$) acting on the phase space \mathcal{A} and to study its dynamical properties.

In particular, it is worth noting that the lower bounds on the ε -entropy that one can derive imply that the topological entropy of this spatial DS is infinite and, consequently, the classical symbolic dynamics with a finite number of symbols is not adequate to clarify the nature of chaos in [21]. In order to overcome this difficulty, it was suggested by Zelik to use Bernoulli shifts with an infinite number of symbols, belonging to the whole interval $\omega \in [0, 1]$. To be more precise, let us consider the Cartesian product $\mathbb{M}_n := [0, 1]^{\mathbb{Z}^n}$ endowed with the Tikhonov topology. Then, this set can be interpreted as the space of all the functions $v : \mathbb{Z}^n \rightarrow [0, 1]$, endowed with the standard local topology. We define a DS $\{T_l, l \in \mathbb{Z}^n\}$ on \mathbb{M}_n by

$$(T_l v)(m) := v(m + l), \quad v \in \mathbb{M}_n, l, m \in \mathbb{Z}^n \quad [22]$$

Based on this model, the following description of spatial chaos was obtained.

Theorem 4 *Let eqn [8] in $\Omega = \mathbb{R}^n$ possess at least one exponentially unstable spatially homogeneous equilibrium. Then, there exist $\alpha > 0$ and a homeomorphic embedding $\tau : \mathbb{M}_n \rightarrow \mathcal{A}$ such that*

$$T_{\alpha l} \circ \tau(v) = \tau \circ T_l(v), \quad \forall l \in \mathbb{Z}^n, v \in \mathbb{M}_n \quad [23]$$

Thus, the spatial dynamics, restricted to the set $\tau(\mathbb{M}_n)$, is conjugated to the symbolic dynamics on \mathbb{M}_n . Moreover, there exists a dynamical invariant (the so-called mean topological dimension) which is always finite for the spatial DS [22] and strictly positive for the Bernoulli scheme \mathbb{M}_n . So, the embedding [23] clarifies, indeed, the nature of chaos arising in the spatial DS [21].

Spatio-Temporal Chaos

To conclude, we briefly discuss an extension of Theorem 4, which takes into account the temporal modes and, thus, gives a description of the spatio-temporal chaos. In order to do so, we first note

that the spatial DS [21] commutes obviously with the temporal evolution operators $S(t)$ and, consequently, an extended $(n+1)$ -parametric semigroup $\{S(t, h), (t, h) \in \mathbb{R}_+ \times \mathbb{R}^n\}$ acts on the attractor:

$$S(t, h) := S(t) \circ T_h, \quad S(t, h) : \mathcal{A} \rightarrow \mathcal{A} \\ t \in \mathbb{R}_+, \quad h \in \mathbb{R}^n \quad [24]$$

Then, this semigroup (interpreted as a DS with multidimensional times) is responsible for all the spatio-temporal dynamical phenomena in the initial PDE [8] and, consequently, the question of finding adequate dynamical characteristics is of a great interest. Moreover, it is also natural to consider the subsemigroups $S_{V_k}(t, h)$ associated with the k -dimensional planes V_k of the spacetime $\mathbb{R}_+ \times \mathbb{R}^n$, $k < n+1$.

Although finding an adequate description of the dynamics of [24] seems to be an extremely difficult task, some particular results in this direction have already been obtained. Thus, it has been proved by Zelik that the semigroup [24] has finite topological entropy and the entropy of its subsemigroups $S_{V_k}(t, h)$ is usually infinite if $k < n+1$. Moreover (adding a natural transport term of the form $(L, \nabla_x)u$ to eqn [8]), it was proved that the analog of Theorem 4 holds for the subsemigroups $S_{V_n}(t, h)$ associated with the n -dimensional hyperplanes V_n of the spacetime. Thus, the infinite-dimensional Bernoulli shifts introduced in the previous subsection can be used to describe the temporal evolution in unbounded domains as well.

In particular, as a consequence of this embedding, the topological entropy of the initial purely temporal evolution semigroup $S(t)$ is also infinite, which

indicates that (even without considering the spatial directions) we have indeed here essential new levels of dynamical complexity which are not observed in the classical DS theory of ODEs.

See also: Dynamical Systems in Mathematical Physics: An Illustration from Water Waves; Ergodic Theory; Evolution Equations: Linear and Nonlinear; Fractal Dimensions in Dynamics; Inviscid flows; Lyapunov Exponents and Strange Attractors.

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Donaldson Invariants see Gauge Theoretic Invariants of 4-Manifolds

Donaldson–Witten Theory

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Introduction

Since they were introduced by Witten in 1988, topological quantum field theories (TQFTs) have had a tremendous impact in mathematical physics (see Birmingham *et al.* (1991) and Cordes *et al.* for a review). These quantum field theories are

constructed in such a way that the correlation functions of certain operators provide topological invariants of the spacetime manifold where the theory is defined. This means that one can use the methods and insights of quantum field theory in order to obtain information about topological invariants of low-dimensional manifolds.

Historically, the first TQFT was Donaldson–Witten theory, also called topological Yang–Mills theory. This theory was constructed by Witten (1998) starting from $\mathcal{N}=2$ super Yang–Mills by a procedure called

“topological twisting.” The resulting model is topological and the famous Donaldson invariants of 4-manifolds are then recovered as certain correlation functions in the topological theory. The analysis of Witten (1998) did not indicate any new method to compute the invariants, but in 1994 the progress in understanding the nonperturbative dynamics of $\mathcal{N}=2$ theories (Seiberg and Witten 1994 a, b) led to an alternative way of computing correlation functions in Donaldson–Witten theory. As Witten (1994) showed, Donaldson–Witten theory can be reduced to another, simpler topological theory consisting of a twisted abelian gauge theory coupled to spinor fields. This theory leads to a different set of 4-manifold invariants, the so-called “Seiberg–Witten invariants,” and Donaldson invariants can be expressed in terms of these invariants through Witten’s “magic formula.” The connection between Seiberg–Witten and Donaldson invariants was streamlined and extended by Moore and Witten by using the so-called u -plane integral (Moore and Witten 1998). This has led to a rather complete understanding of Donaldson–Witten theory from a physical point of view.

In this article we provide a brief review of Donaldson–Witten theory. First, we describe the construction of the model, from both a mathematical and a physical point of view, and state the main results for the Donaldson–Witten generating functional. In the next section, we present the basic results of the u -plane integral of Moore and Witten and sketch how it can be used to solve Donaldson–Witten theory. In the final section, we mention some generalizations of the basic framework. For a complete exposition of Donaldson–Witten theory, the reader is referred to the book by Labastida and Mariño (2005). A short review of the u -plane integral can be found in Mariño and Moore (1998a).

Donaldson–Witten Theory: Basic Construction and Results

Donaldson–Witten Theory According to Donaldson

Donaldson theory as formulated in Donaldson (1990), Donaldson and Kronheimer (1990), and Friedman and Morgan (1991) starts with a principal $G = \mathrm{SO}(3)$ bundle $V \rightarrow X$ over a compact, oriented, Riemannian 4-manifold X , with fixed instanton number k and Stiefel–Whitney class $w_2(V)$ ($\mathrm{SO}(3)$ bundles on a 4-manifold are classified up to isomorphism by these topological data). The moduli space of anti-self-dual (ASD) connections is then defined as

$$\mathcal{M}_{\mathrm{ASD}} = \{A : F^+(A) = 0\} / \mathcal{G} \quad [1]$$

where $F^+(A)$ is the self-dual part of the curvature, and \mathcal{G} is the group of gauge transformations. To construct the Donaldson polynomials, one considers the universal bundle

$$P = (V \times \mathcal{A}^*) / (\mathcal{G} \times G) \quad [2]$$

where \mathcal{A}^* is the space of irreducible G -connections on V . This is a G -bundle over $B^* \times X$, where $B^* = \mathcal{A}^* / \mathcal{G}$ is the space of irreducible connections modulo gauge transformations, and as such has a Pontrjagin class

$$p_1(P) \in H^*(B^*) \otimes H^*(X) \quad [3]$$

One can then obtain differential forms on B^* by taking the slant product of $p_1(P)$ with homology classes in X . In this way we obtain the Donaldson map:

$$\mu : H_i(X) \longrightarrow H^{4-i}(B^*) \quad [4]$$

After restriction to $\mathcal{M}_{\mathrm{ASD}}$, we obtain the following differential forms on the moduli space of ASD connections:

$$\begin{aligned} x \in H_0(X) &\rightarrow \mathcal{O}(x) \in H^4(\mathcal{M}_{\mathrm{ASD}}) \\ S \in H_2(X) &\rightarrow I_2(S) \in H^2(\mathcal{M}_{\mathrm{ASD}}) \end{aligned} \quad [5]$$

If the manifold X has $b_1(X) \neq 0$, there are also cohomology classes associated to 1-cycles and 3-cycles, but we will not consider them here.

We can now formally define the Donaldson invariants as follows. Consider the space

$$A(X) = \mathrm{Sym}(H_0(X) \oplus H_2(X)) \quad [6]$$

with a typical element written as $x^\ell S_{i_1} \cdots S_{i_p}$. The Donaldson invariant corresponding to this element of $A(X)$ is the following intersection number:

$$\begin{aligned} \mathcal{D}_X^{w_2(V), k}(x^\ell S_{i_1} \cdots S_{i_p}) \\ = \int_{\mathcal{M}_{\mathrm{ASD}}} \mathcal{O}^\ell \wedge I_2(S_{i_1}) \wedge \cdots \wedge I_2(S_{i_p}) \end{aligned} \quad [7]$$

where $\mathcal{M}_{\mathrm{ASD}}$ is the moduli space of ASD connections with second Stiefel–Whitney class $w_2(V)$ and instanton number k . The integral in [7] will be different from zero only if the degrees of the forms add up to $\dim(\mathcal{M}_{\mathrm{ASD}})$.

It is very convenient to pack all Donaldson invariants in a generating functional. Let $\{S_i\}_{i=1, \dots, b_2}$ be a basis of 2-cycles. We introduce the formal sum

$$S = \sum_{i=1}^{b_2} v_i S_i \quad [8]$$

where v_i are complex numbers. We then define the Donaldson–Witten generating functional as

$$Z_{\text{DW}}^{w_2(V)}(p, v_i) = \sum_{k=0}^{\infty} \mathcal{D}_X^{w_2(V), k}(e^{pX+S}) \quad [9]$$

where on the right-hand side we are summing over all instanton numbers, that is, we are summing over all topological configurations of the $\text{SO}(3)$ gauge field with a fixed $w_2(V)$. This gives a formal power series in p and v_i .

For $b_2^+(X) > 1$, the generating functional [9] is a diffeomorphism invariant of X ; therefore, it is potentially a powerful tool in four-dimensional topology. When $b_2^+(X) = 1$, Donaldson invariants are metric dependent. The metric dependence can be described in more detail as follows. Define the period point as the harmonic 2-form satisfying

$$*\omega = \omega, \quad \omega^2 = 1 \quad [10]$$

which depends on the conformal class of the metric. As the conformal class of the metric varies, ω describes a curve in the cone

$$V_+ = \{\omega \in H^2(X, \mathbf{R}) : \omega^2 > 0\} \quad [11]$$

Let $\zeta \in H^2(X)$ satisfy

$$\zeta \equiv w_2(V) \bmod 2, \quad \zeta^2 < 0, \quad (\zeta, \omega) = 0 \quad [12]$$

Such an element ζ defines a “wall” in V_+ :

$$W_\zeta = \{\omega : (\zeta, \omega) = 0\} \quad [13]$$

The complements of these walls are called “chambers,” and the cone V_+ is then divided in chambers separated by walls. A class ζ satisfying [12] is the first Chern class associated to a reducible solution of the ASD equations, and it causes a singularity in moduli space: the Donaldson invariants jump when we pass through such a wall. Therefore, when $b_2^+(X) = 1$, Donaldson invariants are metric independent in each chamber. A basic problem in Donaldson–Witten theory is to determine the jump in the generating function as we cross a wall,

$$Z_+^\zeta(p, S) - Z_-^\zeta(p, S) = WC_\zeta(p, S) \quad [14]$$

The jump term $WC_\zeta(p, S, \delta)$ is usually called the “wall-crossing” term.

The basic goal of Donaldson theory is to study the properties of the generating functional [9] and to compute it for different 4-manifolds X . On the mathematical side, many results have been obtained on Z_{DW} , and some of them can be found in Donaldson and Kronheimer (1990), Friedman and Morgan (1991), Stern (1998), and Göttsche

(1996). On the other hand, Donaldson theory can be formulated as a topological field theory, and many of these results can be obtained by using quantum field theory techniques. This will be our main focus for the rest of the article.

Donaldson–Witten Theory According to Witten

Witten (1988) constructed a twisted version of $\mathcal{N} = 2$ super Yang–Mills theory which has a nilpotent Becchi–Rouet–Stora–Tyutin (BRST) charge (modulo gauge transformations)

$$\bar{Q} = \epsilon^{\dot{\alpha}A} Q_{\dot{\alpha}A} \quad [15]$$

where $Q_{\dot{\alpha}A}$ are the supersymmetric (SUSY) charges. Here $\dot{\alpha}$ is a chiral spinor index and A has its origin in the $\text{SU}(2)$ \mathcal{R} -symmetry. The field content of the theory is the standard twisted $\mathcal{N} = 2$ vector multiplet:

$$A, \psi_\mu = \psi_{\alpha\dot{\alpha}}, \phi, \quad D_{\mu\nu}^+, \chi_{\mu\nu}^+ = \bar{\psi}_{\dot{\alpha}\beta}, \quad \bar{\phi}, \eta = \bar{\psi}^{\dot{\alpha}}_{\dot{\alpha}} \quad [16]$$

where $(1/2)D_{\mu\nu}^+ dx^\mu dx^\nu$ is a self-dual 2-form derived from the auxiliary fields, etc. All fields are valued in the adjoint representation of the gauge group. After twisting, the theory is well defined on any Riemannian 4-manifold, since the fields are naturally interpreted as differential forms and the \bar{Q} charge is a scalar (Witten 1988).

The observables of the theory are \bar{Q} cohomology classes of operators, and they can be constructed from 0-form observables $\mathcal{O}^{(0)}$ using the descent procedure. This amounts to solving the equations

$$d\mathcal{O}^{(i)} = \{\bar{Q}, \mathcal{O}^{(i+1)}\}, \quad i = 0, \dots, 3 \quad [17]$$

The integration over i -cycles $\gamma^{(i)}$ in X of the operators $\mathcal{O}^{(i)}$ is then an observable. These descent equations have a canonical solution: the 1-form-valued operator $K_{\alpha\dot{\alpha}} = -i\delta_{\alpha}^A Q_{\dot{\alpha}A}/4$ verifies

$$d = \{\bar{Q}, K\} \quad [18]$$

as a consequence of the supersymmetry algebra. The operators $\mathcal{O}^{(i)} = K^i \mathcal{O}^{(0)}$ solve the descent equations [17] and are canonical representatives. When the gauge group is $\text{SU}(2)$, the observables are obtained by the descent procedure from the operator

$$\mathcal{O} = \text{tr}(\phi^2) \quad [19]$$

The topological descendant $\mathcal{O}^{(2)}$ is given by

$$\mathcal{O}^{(2)} = -\frac{1}{2} \text{tr} \left(\frac{1}{\sqrt{2}} \phi (F_{\mu\nu}^- + D_{\mu\nu}^+) - \frac{1}{4} \psi_\mu \psi_\nu \right) dx^\mu \wedge dx^\nu \quad [20]$$

and the resulting observable is

$$I_2(S) = \int_S \mathcal{O}^{(2)} \quad [21]$$

\mathcal{O} and $I_2(S)$ correspond to the cohomology classes in [5]. One of the main results of Witten (1988) is that the semiclassical approximation in the twisted $\mathcal{N}=2$ Yang–Mills theory is exact. The semiclassical evaluation of correlation functions of the observables above leads directly to the definition of Donaldson invariants, and the generating functional [9] can be written as a correlation function of the twisted theory. One then has

$$Z_{\text{DW}}^{w_2(V)}(p, S) = \left\langle \exp(p\mathcal{O} + I_2(S)) \right\rangle \quad [22]$$

Results for the Donaldson–Witten Generating Function

The basic results that have emerged from the physical approach to Donaldson–Witten theory are the following.

1. The Donaldson–Witten generating functional is in general the sum of the two terms,

$$Z_{\text{DW}} = Z_u + Z_{\text{SW}} \quad [23]$$

(We have omitted the Stiefel–Whitney class for convenience.) The first term, Z_u , is called the “ u -plane integral.” It is given by a complicated integral over \mathbb{C} which can be written, in turn, as an integral over a fundamental domain of the congruence subgroup $\Gamma^0(4)$ of $\text{SL}(2, \mathbb{Z})$. Z_u depends only on the cohomology ring of X , and therefore does not contain any information beyond the one provided by classical topology. Finally, Z_u vanishes if $b_2^+(X) > 1$, and it is responsible for the wall-crossing behavior of Z_{DW} when $b_2^+(X) = 1$.

2. The second term of [23], Z_{SW} , is called the Seiberg–Witten contribution. This contribution involves the Seiberg–Witten invariants of X , which are obtained by considering the moduli problem defined by the Seiberg–Witten monopole equations (Witten 1994b):

$$\begin{aligned} F_{\dot{\alpha}\dot{\beta}}^+ + 4i\bar{M}_{(\dot{\alpha}}M_{\dot{\beta})} &= 0 \\ D_L^{\alpha\dot{\alpha}}M_{\dot{\alpha}} &= 0 \end{aligned} \quad [24]$$

In these equations, $M_{\dot{\alpha}}$ is a section of the spinor bundle $S^+ \otimes L^{1/2}$, L is the determinant line bundle of a Spin_c structure on X , $F_{\dot{\alpha}\dot{\beta}}^+ = \bar{\sigma}^{\mu\nu}_{\dot{\alpha}\dot{\beta}} F_{\mu\nu}^+$ is the self-dual part of the curvature of a $\text{U}(1)$ connection on L , and D_L is the Dirac operator for the bundle $S^+ \otimes L^{1/2}$. The solutions of these equations modulo gauge equivalence form the moduli space $\mathcal{M}_S W$, and the Seiberg–Witten invariants are defined by integrating suitable differential forms on this moduli

space. We will label Spin_c structures by the class $\lambda = c_1(L^{1/2}) \in H^2(X, \mathbb{Z}) + w_2(X)/2$. We say that λ is a Seiberg–Witten basic class if the corresponding Seiberg–Witten invariants are not all zero. If $\mathcal{M}_S W$ is zero dimensional, the Seiberg–Witten invariant depends only on the Spin_c structure associated to $\lambda = c_1(L^{1/2})$, and is denoted by $\text{SW}(\lambda)$.

3. A manifold X is said to be of Seiberg–Witten simple type if all the Seiberg–Witten basic classes have a zero-dimensional moduli space. For simply connected 4-manifolds of Seiberg–Witten simple type and with $b_2^+(X) > 1$, Witten determined the Seiberg–Witten contribution and proposed the following “magic formula” for Z_{DW} (Witten 1994b):

$$\begin{aligned} Z_{\text{DW}} = 2^{1+7\chi/4+11\sigma/4} \sum_{\lambda} e^{2i\pi(\lambda_0 \cdot \lambda + \lambda_0^2)} \left[e^{2p+S^2/2} e^{2(S, \lambda)} \right. \\ \left. + i^{\chi_h - w_2(V)^2} e^{-2p - S^2/2} e^{-2i(S, \lambda)} \right] \text{SW}(\lambda) \end{aligned} \quad [25]$$

In this equation, χ, σ are the Euler characteristic and signature of X , respectively, $\chi_h = (\chi + \sigma)/4$ is the holomorphic Euler characteristic of X , and λ_0 is an integer lifting of $w_2(V)$. This formula generalizes previous results by Witten (1994a) for Kähler manifolds. It also follows from this formula that the Donaldson–Witten generating function of simply connected 4-manifolds of Seiberg–Witten simple type and with $b_2^+(X) > 1$ satisfies

$$\left(\frac{\partial^2}{\partial p^2} - 4 \right) Z_{\text{DW}} = 0$$

which is the Donaldson simple type condition introduced by Kronheimer and Mrowka (1994).

4. Using the u -plane integral, one can find explicit expressions for Z_{DW} in more general situations (like non-simply-connected manifolds or manifolds which are not of Seiberg–Witten simple type).

In the next section we explain the formalism of the u -plane integral introduced by Moore and Witten (1998), which makes possible a detailed derivation of the above results.

The u -Plane Integral

Definition of the u -Plane Integral

The evaluation of the Donaldson–Witten generating function can be made by using the results of Seiberg and Witten (1994 a, b) on the low-energy dynamics of $\text{SU}(2)$, $\mathcal{N}=2$ Yang–Mills theory. In their work, Seiberg and Witten determined the exact low-energy effective action of the model up to two derivatives.

From a physical point of view, there are certainly corrections to this effective action which are difficult to evaluate. Fortunately, the computation in the twisted version of the theory can be done by just considering the Seiberg–Witten effective action. This is because the correlation functions in the twisted theory are invariant under rescalings of the metric, so we can evaluate them in the limit of large distances or equivalently of very low energies. The effective action up to two derivatives is sufficient for that purpose.

One way of describing the main result of the work of Seiberg and Witten is that the moduli space of \bar{Q} -fixed points of the twisted $SO(3)$ $\mathcal{N}=2$ theory on a compact 4-manifold has two branches, which we refer to as the Coulomb and Seiberg–Witten branches. On the Coulomb branch the expectation value

$$u = \frac{\langle \text{tr } \phi^2 \rangle}{16\pi^2}$$

breaks $SO(3) \rightarrow U(1)$ via the standard Higgs mechanism. The Coulomb branch is simply a copy of the complex u -plane. The low-energy effective theory on this branch is simply the abelian $\mathcal{N}=2$ gauge theory. However, at two points, $u = \pm 1$, there is a singularity where the moduli space meets a second branch, the Seiberg–Witten branch. At these points, the effective action is given by the magnetic dual of the $U(1)$, $\mathcal{N}=2$ gauge theory coupled to a monopole matter hypermultiplet. Therefore, this branch consists of solutions to the Seiberg–Witten equations [24].

Since the manifold X is compact, the partition function of the twisted theory is a sum over “all” vacuum states. Equation [23] then follows. In this equation, Z_u comes from “integrating over the u -plane,” while Z_{SW} corresponds to the points $u = \pm 1$. As we stated before, Z_u vanishes for manifolds of $b_2^+(X) > 1$, but once this piece has been determined an argument originally presented at Moore and Witten (1998) allows one to derive the form of Z_{SW} as well for arbitrary $b_2^+(X) \geq 1$.

The computation of Z_u is presented in detail in Moore and Witten (1998). The starting point of the computation is the untwisted low-energy theory, which has been described in detail in Seiberg and Witten (1994 a, b) and Witten (1995). It is an $\mathcal{N}=2$ theory characterized by a prepotential \mathcal{F} which depends on an $\mathcal{N}=2$ vector multiplet. The effective gauge coupling is given by $\tau(a) = \mathcal{F}''(a)$, where a is the scalar component of the vector multiplet. The Euclidean Lagrange density for the u -plane theory can be obtained

simply by twisting the physical theory. It can be written as

$$\begin{aligned} & \frac{i}{6\pi} K^4 \mathcal{F}(a) + \frac{1}{16\pi} \left\{ \bar{Q}, \bar{\mathcal{F}}'' \chi (D + F_+) \right\} \\ & - \frac{i\sqrt{2}}{32\pi} \left\{ \bar{Q}, \bar{\mathcal{F}}' d * \psi \right\} - \frac{\sqrt{2}i}{3 \times 2^5 \pi} \\ & \times \left\{ \bar{Q}, \bar{\mathcal{F}}''' \chi_{\mu\nu} \chi^{\nu\lambda} \chi_\lambda^\mu \right\} \sqrt{g} d^4 x \\ & + \mathcal{A}(u) \text{tr} R \wedge R + \mathcal{B}(u) \text{tr} R \wedge \tilde{R} \end{aligned} \quad [26]$$

where $\mathcal{A}(u), \mathcal{B}(u)$ describe the coupling to gravity, and after integration of the corresponding differential forms we obtain terms proportional to the signature σ and Euler characteristic χ of X . The data of the low-energy effective action can be encoded in an elliptic curve of the form

$$y^2 = x^3 - ux^2 + \frac{1}{4}x \quad [27]$$

and τ is the modulus of the curve. The monodromy group of this curve is $\Gamma^0(4)$. All the quantities involved in the action can be obtained by integrating a certain meromorphic differential on the curve, and they can be expressed in terms of modular forms.

As for the operators, we have $u = \mathcal{O}(P)$ by definition. We may then obtain the 2-observables from the descent procedure. The result is that $I(S) \rightarrow \tilde{I}(S) = \int_S K^2 u = \int_S (du/da)(D_+ + F_-) + \dots$. Here D_+ is the auxiliary field. Although one has $I(S) \rightarrow \tilde{I}(S)$ in going from the microscopic theory to the effective theory, it does not necessarily follow that $I(S_1)I(S_2) \rightarrow \tilde{I}(S_1)\tilde{I}(S_2)$ because there can be contact terms. If S_1 and S_2 intersect, then in passing to the low-energy theory we integrate out massive modes. This can induce delta function corrections to the operator product expansion modifying the mapping to the low-energy theory as follows:

$$\exp(I(S)) \rightarrow \exp(\tilde{I}(S) + S^2 T(u)) \quad [28]$$

where $T(u)$ is the contact term. Such contact terms were observed in Witten (1994a) and studied in detail in Losev *et al.* (1998). It can be shown that

$$T(u) = -\frac{1}{24} E_2(\tau) \left(\frac{du}{da} \right)^2 + \frac{1}{3} u \quad [29]$$

where $E_2(\tau)$ is Eisenstein’s series and da/du is one of the periods of the elliptic curve [27].

The final result of Moore and Witten is the following expression:

$$Z_u(p, S) = \int_C \frac{du d\bar{u}}{y^{1/2}} \mu(\tau) e^{2pu + S^2 \tilde{T}(u)} \Psi \quad [30]$$

Here,

$$\begin{aligned}\mu(\tau) &= \frac{d\bar{\tau}}{d\bar{u}} \left(\frac{da}{du} \right)^{1-(1/2)\chi} \Delta^{\sigma/8} \\ \hat{T}(u) &= T(u) + \frac{(du/da)^2}{8\pi y}\end{aligned}\quad [31]$$

where $y = \text{Im } \tau$ and Δ is the discriminant of the curve [27]. The quantity Ψ is essentially a Narain–Siegel theta function associated to the lattice $H^2(X, \mathbb{Z})$. Notice that this lattice is Lorentzian and has signature $(1, (-1)^{b_2^+(X)})$ (since $b_2^+(X) = 1$). The self-dual projection of a 2-form λ can be done with the period point ω as $\lambda_+ = (\lambda, \omega)\omega$. The lattice is shifted by half the second Stiefel–Whitney class of the bundle, $w_2(V)$, that is,

$$\Gamma = H^2(X, \mathbb{Z}) + \frac{1}{2}w_2(V)$$

and

$$\begin{aligned}\Psi &= \exp \left[-\frac{1}{8\pi y} \left(\frac{du}{da} \right)^2 S_-^2 \right] e^{2\pi i \lambda_0^2} \sum_{\lambda \in \Gamma} (-1)^{(\lambda - \lambda_0) \cdot w_2(X)} \\ &\quad \times \left[(\lambda, \omega) + \frac{i}{4\pi y} \frac{du}{da}(S, \omega) \right] \\ &\quad \times \exp \left[-i\pi \bar{\tau}(\lambda_+)^2 - i\pi \tau(\lambda_-)^2 - i \frac{du}{da}(S, \lambda_-) \right]\end{aligned}\quad [32]$$

Here, $w_2(X)$ is the second Stiefel–Whitney class of X , and λ_0 is a choice of lifting of $w_2(V)$ to $H^2(X, \mathbb{Z})$. This expression can be extended to the non-simply-connected case (see Mariño and Moore (1999) and Moore and Witten (1998)). The study of the u -plane integral leads to a systematic derivation of many important results in Donaldson–Witten theory. We will discuss in detail two such applications, Göttsche’s wall-crossing formula and Witten’s “magic formula.”

Wall-Crossing Formula

As shown by Moore and Witten, the u -plane integral is well defined and does not depend on the period point (hence on the metric on X) except for discontinuous behavior at walls. There are two kinds of walls, associated, respectively, to the singularities at $u = \infty$ (the semiclassical region of the underlying Yang–Mills theory) and at $u = \pm 1$, given by

$$\begin{aligned}u = \infty: & \lambda_+ = 0, \lambda \in H^2(X, \mathbb{Z}) + \frac{1}{2}w_2(V) \\ u = \pm 1: & \lambda_+ = 0, \lambda \in H^2(X, \mathbb{Z}) + \frac{1}{2}w_2(X)\end{aligned}\quad [33]$$

The first type of walls is precisely the one that appears in Donaldson theory on manifolds of

$b_2^+(X) = 1$. The discontinuity of the u -plane integral at these walls can be easily computed from eqn [33]:

$$\begin{aligned}\text{WC}_{\zeta=2\lambda}(p, S) &= -\frac{i}{2}(-1)^{(\lambda - \lambda_0, w_2(X))} e^{2\pi i \lambda_0^2} \left[q^{-\lambda^2/2} h_\infty(\tau)^{-2} \vartheta_4^\sigma f_\infty^{-1} \right. \\ &\quad \times \exp \{ 2pu_\infty + S^2 T_\infty - i(\lambda, S)/h_\infty \} \Big]_{q^0}\end{aligned}\quad [34]$$

This expression involves the modular forms $h_\infty, f_\infty, u_\infty$, and T_∞ (the subscript ∞ refers to the fact that they are computed at the “electric” frame which is appropriate for the Seiberg–Witten curve at $u \rightarrow \infty$). They can be written in terms of Jacobi theta functions $\vartheta_i(q)$, with $q = e^{2\pi i \tau}$, and their explicit expression is

$$\begin{aligned}h_\infty(q) &= \frac{1}{2} \vartheta_2(q) \vartheta_3(q) \\ f_\infty(q) &= \frac{\vartheta_2(q) \vartheta_3(q)}{2 \vartheta_4^8(q)} \\ u_\infty(q) &= \frac{\vartheta_2^4(q) + \vartheta_3^4(q)}{2(\vartheta_2(q) \vartheta_3(q))^2} \\ T_\infty(q) &= -\frac{1}{24} \frac{E_2(q)}{h_\infty^2(q)} + \frac{1}{3} u_\infty(q)\end{aligned}\quad [35]$$

The subindex q^0 means that in the expansion in q of the modular forms, we pick the constant term. The formula [34] agrees with the formula of Göttsche (1996) for the wall crossing of the Donaldson–Witten generating functional.

The Seiberg–Witten Contribution and Witten’s Magic Formula

At $u = \pm 1$, Z_u jumps at the second type of walls [33], which are called Seiberg–Witten (SW) walls. In fact, these walls are labeled by classes $\lambda \in H^2(X; \mathbb{Z}) + (1/2)w_2(X)$, which correspond to Spin_c structures on X . At these walls, the Seiberg–Witten invariants have wall-crossing behavior. Since the Donaldson polynomials do not jump at SW walls, it must happen that the change of Z_u at $u = \pm 1$ is canceled by the change of Z_{SW} . As shown by Moore and Witten, this actually allows one to obtain a precise expression for Z_{SW} for general 4-manifolds of $b_2^+(X) \geq 1$.

On general grounds, Z_{SW} is given by the sum of the generating functionals at $u = \pm 1$. These involve a magnetic $U(1)$, $\mathcal{N} = 2$ vector multiplet coupled to a hypermultiplet (the monopole field). The twisted

Lagrangian for such a system involves the magnetic prepotential $\tilde{\mathcal{F}}_D(a_D)$, and it can be written as

$$\begin{aligned} \{\bar{Q}, W\} + \frac{i}{16\pi} \tilde{\tau}_D F \wedge F + p(u) \text{tr} R \wedge *R \\ + \ell(u) \text{tr} R \wedge R - \frac{i\sqrt{2} d\tilde{\tau}_D}{32\pi da_D} (\psi \wedge \psi) \wedge F \\ + \frac{i}{3 \times 2^7 \pi} \frac{d^2 \tilde{\tau}_D}{da_D^2} \psi \wedge \psi \wedge \psi \wedge \psi \end{aligned} \quad [36]$$

where $\tilde{\tau}_D = \tilde{\mathcal{F}}_D''(a_D)$. Using the cancellation of wall crossings, one can actually compute the functions $\tilde{\mathcal{F}}_D(a_D)$, $p(u)$, $\ell(u)$ and determine the precise form of the Seiberg–Witten contributions. One finds that a Spin_c structure λ at $u=1$ gives the following contribution to the Donaldson–Witten generating functional:

$$\begin{aligned} Z_{\text{SW}}^{u=1, \lambda} = \frac{\text{SW}(\lambda)}{16} e^{2i\pi(\lambda_0^2 - \lambda_0 \cdot \lambda)} \\ \times \left[q_D^{-\lambda^2/2} \frac{\vartheta_2^{8+\sigma}}{a_D h_M} \left(-2i \frac{a_D}{h_M^2} \right)^{\lambda_h} \right. \\ \left. \times \exp(2pu_M + i(\lambda, S)/h_M + S^2 T_M) \right]_{q_D^0} \quad [37] \end{aligned}$$

Here, a_D , h_M , u_M , and T_M are modular forms that can be expressed as well in terms of Jacobi theta functions $\vartheta_i(q_D)$, where $q_D = \exp(2\pi i \tau_D)$. The subscript M refers to the monopole point, and they are related by an S -transformation to the quantities obtained in the “electric” frame at $u \rightarrow \infty$. Their explicit expression is

$$\begin{aligned} a_D(q_D) &= -\frac{i}{6} \frac{2E_2(q_D) - \vartheta_3^4(q_D) - \vartheta_4^4(q_D)}{\vartheta_3(q_D)\vartheta_4(q_D)} \\ h_M(q_D) &= \frac{1}{2i} \vartheta_3(q_D)\vartheta_4(q_D) \\ u_M(q_D) &= \frac{1}{2} \frac{\vartheta_3^4(q_D) + \vartheta_4^4(q_D)}{(\vartheta_3(q_D)\vartheta_4(q_D))^2} \\ T_M(q) &= -\frac{1}{24} \frac{E_2(q_D)}{h_M^2(q_D)} + \frac{1}{3} u_M(q_D) \end{aligned} \quad [38]$$

The contribution at $u=-1$ is related to the contribution at $u=1$ by a $u \rightarrow -u$ symmetry:

$$Z_{u=-1}(p, S) = e^{-2\pi i \lambda_0^2 (\chi + \sigma)/4} Z_{u=1}(-p, -iS) \quad [39]$$

If the manifold has $b_2^+(X) > 1$ and is of Seiberg–Witten simple type, [37] reduces to

$$\begin{aligned} (-1)^{\chi_h} 2^{1+7\chi/4+11\sigma/4} e^{2p+S^2/2} e^{-2(S, \lambda)} \\ \times e^{2i\pi(\lambda_0^2 - \lambda_0 \cdot \lambda)} \text{SW}(\lambda) \end{aligned} \quad [40]$$

This leads to Witten’s “magic formula” [25] which expresses the Donaldson invariants in terms of Seiberg–Witten invariants.

Other Applications of the u -Plane Integral

The u -plane integral makes possible to derive other results on the Donaldson–Witten generating functional.

The blow-up formula. This relates the function Z_{DW} on X to Z_{DW} on the blown-up manifold \hat{X} . The u -plane integral leads directly to the general blow-up formula of Fintushel and Stern (1996).

Direct evaluations. The u -plane integral can be evaluated directly in many cases, and this leads to explicit formulas for the Donaldson–Witten generating functional of certain 4-manifolds with $b_2^+(X)=1$, on certain chambers, and in terms of modular forms. For example, there are explicit formulas for the Donaldson–Witten generating functional of product ruled surfaces of the form $S^2 \times \Sigma_g$ in the limiting chambers in which S^2 or Σ_g are very small (Moore and Witten 1998, Mariño and Moore 1999). Moore and Witten (1998) have also derived an explicit formula for the Donaldson invariants of \mathbb{CP}^2 in terms of Hurwitz class numbers.

Extensions of Donaldson–Witten Theory

Donaldson–Witten theory is a twisted version of $\text{SU}(2)$, $\mathcal{N}=2$ Yang–Mills theory. The twisting of more general $\mathcal{N}=2$ gauge theories, involving other gauge groups and/or matter content, leads to other topological field theories that give interesting generalizations of Donaldson–Witten theory. We now briefly list some of these extensions and their most important properties.

Higher-rank theories. The extension of Donaldson–Witten to other gauge groups has been studied in detail in Mariño and Moore (1998b) and Losev *et al.* (1998). One can study the higher-rank generalization of the u -plane integral, and as shown in Mariño and Morre (1998b), this leads to a fairly explicit formula for the Donaldson–Witten generating function in the $\text{SU}(N)$ case, for manifolds with $b_2^+ > 1$ and of Seiberg–Witten simple type. Mathematically, higher-rank generalizations of Donaldson theory turn out to be much more complicated, but they can be studied. In particular, higher-rank generalizations of the Donaldson invariants can be defined and computed (Kronheimer 2004), and the results so far agree with the predictions of Mariño and Moore (1998b). Unfortunately it seems that these higher-rank generalizations do not contain new topological information, besides the one encoded in the Seiberg–Witten invariants.

Theories with matter. Twisted $\text{SU}(2)$, $\mathcal{N}=2$ theories with hypermultiplets lead to generalizations of Donaldson–Witten theory involving nonabelian

monopole equations (see Mariño (1997) and Labastida and Mariño (2005) for a review of these models and some of their properties). The u -plane integral leads to explicit formulas for the generating functionals of these theories, which for manifolds of $b_2^+ > 1$ can be written in terms of Seiberg–Witten invariants. Again, no new topological information seems to be encoded in these theories. One can however exploit new physical phenomena arising in the theories with hypermultiplets (in particular, the presence of superconformal points) to obtain new information about the Seiberg–Witten invariants (see Mariño *et al.* (1999) for these developments).

Vafa–Witten theory. The so-called Vafa–Witten theory is a close cousin of Donaldson–Witten theory, and was introduced by Vafa and Witten (1994) as a topological twist of $\mathcal{N}=4$ Yang–Mills theory. In some cases, the partition function of this theory counts the Euler characteristic of the moduli space of instantons on the 4-manifold X . For a review of some properties of this theory, see Lozano (1999).

See also: Duality in Topological Quantum Field Theory; Mathai–Quillen Formalism; Seiberg–Witten Theory; Topological Quantum Field Theory: Overview.

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Duality in Topological Quantum Field Theory

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Introduction

There have been many exciting interactions between physics and mathematics in the past few decades. A prominent role in these interactions has been played by certain field theories, known as topological quantum field theories (TQFTs). These are quantum field theories whose correlation functions are metric independent and, in fact, compute certain mathematical invariants (Birmingham *et al.* 1991, Cordes *et al.* 1996, Labastida and Lozano 1998).

Well-known examples of TQFTs are, in two dimensions, the topological sigma models (Witten 1988a), which are related to Gromov–Witten invariants and enumerative geometry; in three dimensions, Chern–Simons theory (Witten 1989), which is related to knot and link invariants; and in four dimensions, topological Yang–Mills theory (or Donaldson–Witten theory) (Witten 1988b), which is related to the Donaldson invariants. The two- and four-dimensional theories above are examples of cohomological (also Witten-type) TQFTs. As such, they are related to an underlying supersymmetric quantum field theory (the $\mathcal{N}=2$ nonlinear sigma model, and the $\mathcal{N}=2$ supersymmetric Yang–Mills theory, respectively) and there is no difference between the topological and the standard version on flat space. However, when one considers curved spaces, the topological version differs from the supersymmetric theory on flat space in that some of the fields have modified Lorentz transformation properties (spins). This unconventional spin assignment is also known as twisting, and it comes about basically to preserve supersymmetry on curved space. In fact, the twisting gives rise to at least one nilpotent scalar supercharge Q , which is a certain linear combination of the original (spinor) supersymmetry generators.

In these theories the energy momentum tensor is Q -exact, that is,

$$T_{\mu\nu} = \{Q, \Lambda_{\mu\nu}\}$$

for some $\Lambda_{\mu\nu}$, which (barring potential anomalies) leads to the statement that the correlation functions of operators in the cohomology of Q are all metric independent. Furthermore, the corresponding path integrals are localized to field configurations that are annihilated by Q , and this typically leads to some

moduli problem related to the computation of certain mathematical invariants.

On the other hand, in Chern–Simons theory, as a representative of the so-called Schwarz-type topological theories, the topological character is manifest: one starts with an action which is explicitly independent of the metric on the 3-manifold, and thus correlation functions of metric-independent operators are topological invariants as long as quantization does not introduce any undesired metric dependence.

Even though the primary motivation for introducing TQFTs may be to shed light onto awkward mathematical problems, they have proved to be a valuable tool to gain insight into many questions of interest in physics as well. One such question where TQFTs can (and in fact do) play a role is duality. In what follows, an overview of the manifestations of duality is provided in the context of TQFTs.

Duality

The notion of duality is at the heart of some of the most striking recent breakthroughs in physics and mathematics. In broad terms, a duality (in physics) is an equivalence between different (and often complementary) descriptions of the same physical system. The prototypical example is electric–magnetic (abelian) duality. Other, more sophisticated, examples are the various string-theory dualities, such as T -duality (and its more specialized realization, mirror symmetry) and strong/weak coupling S -duality, as well as field theory dualities such as Montonen–Olive duality and Seiberg–Witten effective duality.

Also, the original 't Hooft conjecture, stating that $SU(N)$ gauge theories are equivalent (or dual), at large N , to string theories, has recently been revived by Maldacena (1998) by explicitly identifying the string-theory duals of certain (supersymmetric) gauge theories.

One could wonder whether similar duality symmetries work for TQFTs as well. As noted in the following, this is indeed the case.

In two dimensions, topological sigma models come under two different versions, known as types A and B, respectively, which correspond to the two different ways in which $\mathcal{N}=2$ supersymmetry can be twisted in two dimensions. Computations in each model localize on different moduli spaces and, for a given target manifold, give different results, but it turns out that if one considers mirror pairs of Calabi–Yau manifolds,

computations in one manifold with the A-model are equivalent to computations in the mirror manifold with the B-model.

Also, in three dimensions, a program has been initiated to explore the duality between large N Chern–Simons gauge theory and topological strings, thereby establishing a link between enumerative geometry and knot and link invariants (Gopakumar and Vafa 1998).

Perhaps the most impressive consequences of the interplay between duality and TQFTs have come out in four dimensions, on which we will focus in what follows.

Duality in Twisted $\mathcal{N}=2$ Theories

As mentioned above, topological Yang–Mills theory (or Donaldson–Witten theory) can be constructed by twisting the pure $\mathcal{N}=2$ supersymmetric Yang–Mills theory with gauge group $SU(2)$. This theory contains a gauge field A , a pair of chiral spinors λ_1, λ_2 , and a complex scalar field B . The twisted theory contains a gauge field A , bosonic scalars λ, ϕ , a Grassman-odd scalar η , a Grassman-odd vector ψ , and a Grassman-odd self-dual 2-form χ .

On a 4-manifold X , and for gauge group G , the twisted action has the form

$$\begin{aligned} S = \int_X d^4x \sqrt{g} \operatorname{tr} \bigg(& F^{+2} - i\chi^{\mu\nu} D_\mu \psi_\nu + i\eta D_\mu \psi^\mu \\ & + \frac{1}{4} \phi \{ \chi_{\mu\nu}, \chi^{\mu\nu} \} + \frac{i}{4} \lambda \{ \psi_\mu, \psi^\mu \} - \lambda D_\mu D^\mu \phi \\ & + \frac{i}{2} \phi \{ \eta, \eta \} + \frac{1}{8} [\lambda, \phi]^2 \bigg) \end{aligned} \quad [1]$$

where F^+ is the self-dual part of the Yang–Mills field strength F . The action [1] is invariant under the transformations generated by the scalar supercharge Q :

$$\begin{aligned} \{Q, A_\mu\} &= \psi_\mu, & \{Q, \chi_{\mu\nu}\} &= F_{\mu\nu}^+ \\ \{Q, \psi\} &= d_A \phi, & \{Q, \eta\} &= i[\lambda, \phi] \\ \{Q, \phi\} &= 0, & \{Q, \lambda\} &= \eta \end{aligned} \quad [2]$$

In these transformations, Q^2 is a gauge transformation with gauge parameter ϕ , modulo field equations. Observables are, therefore, related to the G -equivariant cohomology of Q (i.e., the cohomology of Q restricted to gauge invariant operators). Auxiliary fields can be introduced so that the action [1] is Q -exact, that is,

$$S = \{Q, \Lambda\} \quad [3]$$

for Λ a certain functional of the fields of the theory which comes under the name of gauge fermion, a

BRST-inspired terminology which reflects the formal resemblance of topological cohomological field theories with some aspects of the BRST approach to the quantization of gauge theories. Before constructing the topological observables of the theory, we begin by pointing out that for each independent Casimir of the gauge group G it is possible to construct an operator W_0 , from which operators W_i can be defined recursively through the descent equations $\{Q, W_i\} = dW_{i-1}$. For example, for the quadratic Casimir,

$$W_0 = \frac{1}{8\pi^2} \operatorname{tr}(\phi^2) \quad [4]$$

which generates the following family of operators:

$$\begin{aligned} W_1 &= \frac{1}{4\pi^2} \operatorname{tr}(\phi\psi) \\ W_2 &= \frac{1}{4\pi^2} \operatorname{tr} \left(\frac{1}{2} \psi \wedge \psi + \phi \wedge F \right) \\ W_3 &= \frac{1}{4\pi^2} \operatorname{tr}(\psi \wedge F) \end{aligned} \quad [5]$$

Using these one defines the following observables:

$$\mathcal{O}^{(k)} = \int_{\gamma_k} W_k \quad [6]$$

where $\gamma_k \in H_k(X)$ is a k -cycle on the 4-manifold X . The descent equations imply that they are Q -closed and depend only on the homology class of γ_k .

Topological invariants are constructed by taking vacuum expectation values of products of the operators $\mathcal{O}^{(k)}$:

$$\begin{aligned} & \langle \mathcal{O}^{(k_1)} \mathcal{O}^{(k_2)} \dots \mathcal{O}^{(k_p)} \rangle \\ &= \int \mathcal{O}^{(k_1)} \mathcal{O}^{(k_2)} \dots \mathcal{O}^{(k_p)} e^{-S/e^2} \end{aligned} \quad [7]$$

where the integration has to be understood on the space of field configurations modulo gauge transformations, and e is a coupling constant. Standard arguments show that due to the Q -exactness of the action S , the quantities obtained in [7] are independent of e . This implies that the observables of the theory can be obtained either in the weak-coupling limit $e \rightarrow 0$ (also short-distance or ultraviolet regime, since the $\mathcal{N}=2$ theory is asymptotically free), where perturbative methods apply, or in the strong-coupling (also long-distance or infrared) limit $e \rightarrow \infty$, where one is forced to consider a nonperturbative approach.

In the weak-coupling limit one proves that the correlation functions [7] descend to polynomials in the product cohomology of the moduli space of anti-self-dual (ASD) instantons $H_{k_1}(\mathcal{M}_{\text{ASD}}) \times H_{k_2}(\mathcal{M}_{\text{ASD}}) \times \dots \times H_{k_p}(\mathcal{M}_{\text{ASD}})$, which are precisely

the Donaldson polynomial invariants of X . However, the weak-coupling analysis does not add any new ingredient to the problem of the actual computation of the invariants. The difficulties that one has to face in the field theory representation are similar to those in ordinary Donaldson theory.

Nevertheless, the field theory connection is very important since in this theory the strong- and weak-coupling limits are exact, and therefore the door is open to find a strong-coupling description which could lead to a new, simpler representation for the Donaldson invariants.

This alternative strategy was pursued by Witten (1994a), who found the strong-coupling realization of the Donaldson–Witten theory after using the results on the strong-coupling behavior of $\mathcal{N}=2$ supersymmetric gauge theories which he and Seiberg (Seiberg and Witten 1994a–c) had discovered. The key ingredient in Witten’s derivation was to assume that the strong-coupling limit of Donaldson–Witten theory is equivalent to the “sum” over the twisted effective low-energy descriptions of the corresponding $\mathcal{N}=2$ physical theory. This “sum” is not entirely a sum, as in general it has a part which contains a continuous integral. The “sum” is now known as integration over the u -plane after the work of Moore and Witten (1998). Witten’s (1994a) assumption can be simply stated as saying that the weak-/strong-coupling limit and the twist commute. In other words, to study the strong-coupling limit of the topological theory, one first untwists, then works out the strong-coupling limit of the physical theory and, finally, one twists back. From such a viewpoint, the twisted effective (strong-coupling) theory can be regarded as a TQFT dual to the original one. In addition, one could ask for the dual moduli problem associated to this dual TQFT. It turns out that in many interesting situations ($b_2^+(X) > 1$) the dual moduli space is an abelian system corresponding to the Seiberg–Witten or monopole equations (Witten 1994a). The topological invariants associated with this new moduli space are the celebrated Seiberg–Witten invariants.

Generalizations of Donaldson–Witten theory, with either different gauge groups and/or additional matter content (such as, e.g., twisted $\mathcal{N}=2$ Yang–Mills multiplets coupled to twisted $\mathcal{N}=2$ matter multiplets) are possible, and some of the possibilities have in fact been explored (see Moore and Witten (1998) and references therein). The main conclusion that emerges from these analyses is that, in all known cases, the relevant topological information is captured by the Seiberg–Witten invariants, irrespectively of the gauge group and matter content of the theory under consideration. These cases are not reviewed

here, but rather the attention is turned to the twisted theories which emerge from $\mathcal{N}=4$ supersymmetric gauge theories.

Duality in Twisted $\mathcal{N}=4$ Theories

Unlike the $\mathcal{N}=2$ supersymmetric case, the $\mathcal{N}=4$ supersymmetric Yang–Mills theory in four dimensions is unique once the gauge group G is fixed. The microscopic theory contains a gauge or gluon field, four chiral spinors (the gluinos) and six real scalars. All these fields are massless and take values in the adjoint representation of the gauge group. The theory is finite and conformally invariant, and is conjectured to have a duality symmetry exchanging strong and weak coupling and exchanging electric and magnetic fields, which extends to a full $SL(2, \mathbb{Z})$ symmetry acting on the microscopic complexified coupling (Montonen and Olive 1977)

$$\tau = \frac{\theta}{2\pi} + \frac{4\pi i}{e^2} \quad [8]$$

As in the $\mathcal{N}=2$ case, the $\mathcal{N}=4$ theory can be twisted to obtain a topological model, only that, in this case, the topological twist can be performed in three inequivalent ways, giving rise to three different TQFTs (Vafa and Witten 1994). A natural question to answer is whether the duality properties of the $\mathcal{N}=4$ theory are shared by its twisted counterparts and, if so, whether one can take advantage of the calculability of topological theories to shed some light on the behavior and properties of duality.

The answer is affirmative, but it is instructive to clarify a few points. First, as mentioned above, the topological observables in twisted $\mathcal{N}=2$ theories are independent of the coupling constant e , so the question arises as to how the twisted $\mathcal{N}=4$ theories come to depend on the coupling constant. As it turns out, twisted $\mathcal{N}=2$ supersymmetric gauge theories have an off-shell formulation such that the TQFT action can be expressed as a Q -exact expression, where Q is the generator of the topological symmetry. Actually, this is true only up to a topological θ -term $\int_X \text{tr}(F \wedge F)$,

$$S = \frac{1}{2e^2} \int_X \sqrt{g} d^4x \{Q, \Lambda\} - 2\pi i \tau \frac{1}{16\pi^2} \int_X \text{tr}(F \wedge F) \quad [9]$$

for some Λ . However, the $\mathcal{N}=2$ supersymmetric gauge theories possess a global $U(1)$ chiral symmetry which is generically anomalous, so one can actually

get rid of the θ -term with a chiral rotation. As a result of this, the observables in the topological theory are insensitive to θ -terms (and hence to τ and e) up to a rescaling.

On the other hand, in $\mathcal{N}=4$ supersymmetric gauge theories θ -terms are observable. There is no chiral anomaly and these terms cannot be shifted away as in the $\mathcal{N}=2$ case. This means that in the twisted theories one might have a dependence on the coupling constant τ , and that – up to anomalies – this dependence should be holomorphic (resp. antiholomorphic if one reverses the orientation of the 4-manifold). In fact, on general grounds, one would expect for the partition functions of the twisted theories on a 4-manifold X and for gauge group G to take the generic form

$$Z_X(G) = q^{-c(X,G)} \sum_k q^k \chi(\mathcal{M}_k) \quad [10]$$

where $q = e^{2\pi i \tau}$, c is a universal constant (depending on X and G), $k = (1/16\pi^2) \int_X \text{tr}(F \wedge F)$ is the instanton number, and $\chi(\mathcal{M}_k)$ encodes the topological information corresponding to a sector of the moduli space of the theory with instanton number k .

Now we can be more precise as to how we expect to see the Montonen–Olive duality in the twisted $\mathcal{N}=4$ theories. First, under $\tau \rightarrow -1/\tau$ the gauge group G gets exchanged with its dual group \hat{G} . Correspondingly, the partition functions should behave as modular forms

$$Z_G(-1/\tau) = \pm \kappa(X, G) \tau^w Z_{\hat{G}}(\tau) \quad [11]$$

where κ is a constant (depending on X and G), and the modular weight w should depend on X in such a way that it vanishes on flat space.

In addition to this, in the $\mathcal{N}=4$ theory all the fields take values in the adjoint representation of G . Hence, if $H^2(X, \pi_1(G)) \neq 0$, it is possible to consider nontrivial $G/\text{Center}(G)$ gauge configurations with discrete magnetic 't Hooft flux through the 2-cycles of X . In fact, $G/\text{Center}(G)$ bundles on X are classified by the instanton number and a characteristic class $\nu \in H^2(X, \pi_1(G))$. For example, if $G = \text{SU}(2)$, we have $\hat{G} = \text{SU}(2)/\mathbb{Z}_2 = \text{SO}(3)$ and ν is the second Stiefel–Whitney class $w_2(E)$ of the gauge bundle E . This Stiefel–Whitney class can be represented in de Rham cohomology by a class in $H^2(X, \mathbb{Z})$ defined modulo 2, that is, $w_2(E)$ and $w_2(E) + 2\omega$, with $\omega \in H^2(X, \mathbb{Z})$, represent the same 't Hooft flux, so if $w_2(E) = 2\lambda$, for some $\lambda \in H^2(X, \mathbb{Z})$, then the gauge configuration is trivial in $\text{SO}(3)$ (it has no 't Hooft flux).

Similarly, for $G = \text{SU}(N)$ (for which $\hat{G} = \text{SU}(N)/\mathbb{Z}_N$), one can fix fluxes in $H^2(X, \mathbb{Z}_N)$ (the

corresponding Stiefel–Whitney class is defined modulo N). One has, therefore, a family of partition functions $Z_\nu(\tau)$, one for each magnetic flux ν . The $\text{SU}(N)$ partition function is obtained by considering the zero flux partition function (up to a constant factor), while the (dual) $\text{SU}(N)/\mathbb{Z}_N$ partition function is obtained by summing over all ν , and both are to be exchanged under $\tau \rightarrow -1/\tau$. The action of $\text{SL}(2, \mathbb{Z})$ on the Z_ν should be compatible with this exchange, and thus the $\tau \rightarrow -1/\tau$ operation mixes the Z_ν by a discrete Fourier transform which, for $G = \text{SU}(N)$ reads

$$Z_\nu(-1/\tau) = \pm \kappa(X, G) \tau^w \sum_u e^{2\pi i u \cdot \nu / N} Z_u(\tau) \quad [12]$$

We are now in a position to examine the (three) twisted theories in some detail. For further details and references, the reader is referred to Lozano (1999).

The first twisted theory considered here possesses only one scalar supercharge (and hence comes under the name of “half-twisted theory”). It is a nonabelian generalization of the Seiberg–Witten abelian monopole theory, but with the monopole multiplets taking values in the adjoint representation of the gauge group. The theory can be perturbed by giving masses to the monopole multiplets while still retaining its topological character. The resulting theory is the twisted version of the mass-deformed $\mathcal{N}=4$ theory, which preserves $\mathcal{N}=2$ supersymmetry and whose low-energy effective description is known. This connection with $\mathcal{N}=2$ theories, and its topological character, makes it possible to go to the long-distance limit and compute in terms of the twisted version of the low-energy effective description of the supersymmetric theory. Below, we review how the u -plane approach works for gauge group $\text{SU}(2)$.

The twisted theory for gauge group $\text{SU}(2)$ has a $\text{U}(1)$ global symmetry (the ghost number) which has an anomaly $-3(2\chi + 3\sigma)/4$ on gravitational backgrounds (i.e., on curved manifolds). Nontrivial topological invariants are thus obtained by considering the vacuum expectation value of products of observables with ghost numbers adding up to $-3(2\chi + 3\sigma)/4$. The relevant observables for this theory and gauge group $\text{SU}(2)$ or $\text{SO}(3)$ are precisely the same as in the Donaldson–Witten theory (eqns [4] and [5]). In addition to this, it is possible to enrich the theory by including sectors with nontrivial nonabelian electric and magnetic 't Hooft fluxes which, as pointed out above, should behave under $\text{SL}(2, \mathbb{Z})$ duality in a well-defined fashion.

The generating function for these correlation functions is given as an integration over the moduli space of vacua of the physical theory (the u -plane), which, for generic values of the mass parameter, forms a one-dimensional complex compact manifold (described by a complex variable customarily denoted by u , hence the name), which parametrizes a family of elliptic curves that encodes all the relevant information about the low-energy effective description of the theory. At a generic point in the moduli space of vacua, the only contribution to the topological correlation functions comes from a twisted $\mathcal{N}=2$ abelian vector multiplet. Additional contributions come from points in the moduli space where the low-energy effective description is singular (i.e., where the associated elliptic curve degenerates).

Therefore, the total contribution to the generating function thus consists of an integration over the moduli space with the singularities removed – which is nonvanishing for $b_2^+(X)=1$ (Moore and Witten 1998) only – plus a discrete sum over the contributions of the twisted effective theories at each of the three singularities of the low-energy effective description (Seiberg and Witten 1994a, b, c). The effective theory at a given singularity contains, together with the appropriate dual photon multiplet, one charged hypermultiplet, which corresponds to the state becoming massless at the singularity. The complete effective action for these massless states also contains certain measure factors and contact terms among the observables, which reproduce the effect of the massive states that have been integrated out as well as incorporate the coupling to gravity (i.e., explicit nonminimal couplings to the metric of the 4-manifold). How to determine these *a priori* unknown functions was explained in Moore and Witten (1998). The idea is as follows. At points on the u -plane where the (imaginary part of the) effective coupling diverges, the integral is discontinuous at anti-self-dual abelian gauge configurations. This is commonly referred to as “wall crossing.” Wall crossing can take place at the singularities of the moduli space – the appropriate local effective coupling τ_{eff} diverges there – and, in the case of the asymptotically free theories, at the point at infinity – the effective electric coupling diverges owing to asymptotic freedom.

On the other hand, the final expression for the invariants can exhibit a wall-crossing behavior at most at $u \rightarrow \infty$, so the contribution to wall crossing from the integral at the singularities at finite values of u must cancel against the contributions coming from the effective theories there, which also display wall-crossing discontinuities. Imposing this

cancellation fixes almost completely the unknown functions in the contributions to the topological correlation functions from the singularities. The final result for the contributions from the singularities (which give the complete answer for the correlation functions when $b_2^+(X) > 1$) is written explicitly and completely in terms of the fundamental periods da/du (written in the appropriate local variables) and the discriminant of the elliptic curve comprising the Seiberg–Witten solution for the physical theory. For simply connected spin 4-manifolds of simple type the generating function is given by

$$\begin{aligned} \langle e^{p\mathcal{O}+I(S)} \rangle_\nu &= 2^{(\nu/2+(2\chi+3\sigma)/8)} m^{-(3\nu+7\sigma)/8} (\eta(\tau))^{-12\nu} \\ &\times \left\{ (\kappa_1)^\nu \left(\frac{da}{du} \right)_1^{-(\nu+\sigma/4)} e^{2pu_1+S^2T_1} \right. \\ &\times \sum_x \delta_{[x/2],\nu} n_x e^{(i/2)(du/da)_1 x \cdot S} \\ &+ 2^{-b_2/2} (-1)^{\sigma/8} (\kappa_2)^\nu \left(\frac{da}{du} \right)_2^{-(\nu+\sigma/4)} \\ &\times e^{2pu_2+S^2T_2} \sum_x (-1)^{\nu \cdot x/2} n_x e^{(i/2)(du/da)_2 x \cdot S} \\ &+ 2^{-b_2/2} i^{-\nu^2} (\kappa_3)^\nu \left(\frac{da}{du} \right)_3^{-(\nu+\sigma/4)} e^{2pu_3+S^2T_3} \\ &\left. \times \sum_x (-1)^{\nu \cdot x/2} n_x e^{(i/2)(du/da)_3 x \cdot S} \right\} \quad [13] \end{aligned}$$

where x is a Seiberg–Witten basic class (and n_x is the corresponding Seiberg–Witten invariant), m is the mass parameter of the theory, $\nu = (\chi + \sigma)/4$, $\nu \in H^2(X, \mathbb{Z}_2)$ is a ’t Hooft flux, S is the formal sum $S = \sum_a \alpha_a \Sigma_a$ (and, correspondingly, $I(S) = \sum_a \alpha_a I(\Sigma_a)$, with $I(\Sigma_a) = \int_{\Sigma_a} W_2$), where $\{\Sigma_a\}_{a=1,\dots,b_2(X)}$ form a basis of $H_2(X)$ and α_a are constant parameters, while $\eta(\tau)$ is the Dedekind function, $\kappa_i = (du/dq_{\text{eff}})_{u=u_i}$ (with $q_{\text{eff}} = \exp(2\pi i \tau_{\text{eff}})$, and τ_{eff} is the ratio of the fundamental periods of the elliptic curve), and the contact terms T_i have the form

$$T_i = -\frac{1}{12} \left(\frac{du}{da} \right)_i^2 + E_2(\tau) \frac{u_i}{6} + \frac{m^2}{72} E_4(\tau) \quad [14]$$

with E_2 and E_4 the Einstein series of weights 2 and 4, respectively. Evaluating the quantities in [13] gives the final result as a function of the physical parameters τ and m , and of topological data of X as the Euler characteristic χ , the signature σ and the basic classes x . The expression [13] has to be understood as a formal power series in p and α_a , whose coefficients give the vacuum expectation values of products of $\mathcal{O} = W_0$ and $I(\Sigma_a)$.

The generating function [13] has nice properties under the modular group. For the partition function Z_v ,

$$\begin{aligned} Z_v(\tau + 1) &= (-1)^{\sigma/8} i^{-v^2} Z_v(\tau) \\ Z_v(-1/\tau) &= 2^{-b_2/2} (-1)^{\sigma/8} \left(\frac{\tau}{i}\right)^{-\chi/2} \\ &\quad \times \sum_w (-1)^{w \cdot v} Z_w(\tau) \end{aligned} \quad [15]$$

Also, with $Z_{\text{SU}(2)} = 2^{-1} Z_{v=0}$ and $Z_{\text{SO}(3)} = \sum_v Z_v$,

$$\begin{aligned} Z_{\text{SU}(2)}(\tau + 1) &= (-1)^{\sigma/8} Z_{\text{SU}(2)}(\tau) \\ Z_{\text{SO}(3)}(\tau + 2) &= Z_{\text{SO}(3)}(\tau) \\ Z_{\text{SU}(2)}(-1/\tau) &= (-1)^{\sigma/8} 2^{-\chi/2} \tau^{-\chi/2} Z_{\text{SO}(3)}(\tau) \end{aligned} \quad [16]$$

Notice that the last of these three equations corresponds precisely to the strong–weak coupling duality transformation conjectured by Montonen and Olive (1977).

As for the correlation functions, one finds the following behavior under the inversion of the coupling:

$$\begin{aligned} \left\langle \frac{1}{8\pi^2} \text{tr} \phi^2 \right\rangle_{\tau}^{\text{SU}(2)} &= \langle \mathcal{O} \rangle_{\tau}^{\text{SU}(2)} = \frac{1}{\tau^2} \langle \mathcal{O} \rangle_{-1/\tau}^{\text{SO}(3)} \\ \left\langle \frac{1}{8\pi^2} \int_S \text{tr}(2\phi F + \psi \wedge \psi) \right\rangle_{\tau}^{\text{SU}(2)} &= \langle I(S) \rangle_{\tau}^{\text{SU}(2)} \\ &= \frac{1}{\tau^2} \langle I(S) \rangle_{-1/\tau}^{\text{SO}(3)} \\ \langle I(S) I(S) \rangle_{\tau}^{\text{SU}(2)} &= \left(\frac{\tau}{i}\right)^{-4} \langle I(S) I(S) \rangle_{-1/\tau}^{\text{SO}(3)} \\ &\quad + \frac{i}{2\pi \tau^3} \langle \mathcal{O} \rangle_{-1/\tau}^{\text{SO}(3)} \#(S \cap S) \end{aligned} \quad [17]$$

Therefore, as expected, the partition function of the twisted theory transforms as a modular form, while the topological correlation functions turn out to transform covariantly under $\text{SL}(2, \mathbb{Z})$, following a pattern which can be reproduced with a far more simple topological abelian model.

The second example considered next is the Vafa–Witten (1994) theory. This theory possesses two scalar supercharges, and has the unusual feature that the virtual dimension of its moduli space is exactly zero (it is an example of balanced TQFT), and therefore the only nontrivial topological observable is the partition function itself. Furthermore, the twisted theory does not contain spinors, so it is well defined on any compact, oriented 4-manifold.

Now this theory computes, with the subtleties explained in Vafa and Witten (1994), the Euler characteristic of instanton moduli spaces. In fact, in this case in the generic partition function [10],

$$Z_X(G) = q^{-c(X,G)} \sum_k q^k \chi(\mathcal{M}_k) \quad [18]$$

$\chi(\mathcal{M}_k)$ is the Euler characteristic of a suitable compactification of the k th instanton moduli space \mathcal{M}_k of gauge group G in X .

As in the previous example, it is possible to consider nontrivial gauge configurations in $G/\text{Center}(G)$ and compute the partition function for a fixed value of the 't Hooft flux $v \in H^2(X, \pi_1(G))$. In this case, however, the Seiberg–Witten approach is not available, but, as conjectured by Vafa and Witten, one can nevertheless carry out computations in terms of the vacuum degrees of freedom of the $\mathcal{N}=1$ theory which results from giving bare masses to all the three chiral multiplets of the $\mathcal{N}=4$ theory. It should be noted that a similar approach was introduced by Witten (1994b) to obtain the first explicit results for the Donaldson–Witten theory just before the far more powerful Seiberg–Witten approach was available.

As explained in detail by Vafa and Witten (1994), the twisted massive theory is topological on Kähler 4-manifolds with $b^{2,0} \neq 0$, and the partition function is actually invariant under the perturbation. In the long-distance limit, the partition function is given as a finite sum over the contributions of the discrete massive vacua of the resulting $\mathcal{N}=1$ theory. In the case at hand, it turns that, for $G = \text{SU}(N)$, the number of such vacua is given by the sum of the positive divisors of N . The contribution of each vacuum is universal (because of the mass gap), and can be fixed by comparing with known mathematical results (Vafa and Witten 1994). However, this is not the end of the story. In the twisted theory, the chiral superfields of the $\mathcal{N}=4$ theory are no longer scalars, so the mass terms cannot be invariant under the holonomy group of the manifold unless one of the mass parameters be a holomorphic 2-form ω . (Incidentally, this is the origin of the constraint $b^{(2,0)} \neq 0$ mentioned above.) This spatially dependent mass term vanishes where ω does, and we will assume as in Vafa and Witten (1994) and Witten (1994b) that ω vanishes with multiplicity 1 on a union of disjoint, smooth complex curves $C_i, i=1, \dots, n$ of genus g_i which represent the canonical divisor K of X . The vanishing of ω introduces corrections involving K whose precise form is not known *a priori*. In the $G = \text{SU}(2)$ case, each of the $\mathcal{N}=1$ vacua bifurcates along each of the components C_i of the canonical divisor into two strongly coupled massive vacua. This vacuum degeneracy is believed to stem from the spontaneous breaking of a \mathbb{Z}_2 chiral symmetry which is unbroken in bulk (see, e.g., Vafa and Witten (1994) and Witten (1994b)).

The structure of the corrections for $G = \text{SU}(N)$ (see [19] below) suggests that the mechanism at work in this case is not chiral symmetry breaking.

Indeed, near any of the C_i 's, there is an N -fold bifurcation of the vacuum. A plausible explanation for this degeneracy could be found in the spontaneous breaking of the center of the gauge group (which for $G = \text{SU}(N)$ is precisely \mathbb{Z}_N). In any case, the formula for $\text{SU}(N)$ can be computed (at least when N is prime) along the lines explained by Vafa and Witten (1994) and assuming that the resulting partition function satisfies a set of nontrivial constraints which are described below.

Then, for a given 't Hooft flux $\nu \in H^2(X, \mathbb{Z}_N)$, the partition function for gauge group $\text{SU}(N)$ (with prime N) is given by

$$Z_\nu = \left(\sum_{\mathcal{E}} \delta_{\nu, w_N(\mathcal{E})} \prod_{i=1}^n \prod_{\lambda=0}^{N-1} \left(\frac{\chi_\lambda}{\eta} \right)^{(1-g_i)\delta_{\mathcal{E}_i, \lambda}} \right) \times \left(\frac{1}{N^2} G(q^N) \right)^{\nu/2} + N^{1-b_1} \times \sum_{m=0}^{N-1} \left[\prod_{i=1}^n \left(\sum_{\lambda=0}^{N-1} \left(\frac{\chi_{m, \lambda}}{\eta} \right)^{1-g_i} e^{(2i\pi/N)\lambda \nu \cdot [C_i]_N} \right) \right] \times e^{i\pi((N-1)/N)m\nu^2} \left(\frac{G(\alpha^m q^{1/N})}{N^2} \right)^{\nu/2} \quad [19]$$

where $\alpha = \exp(2\pi i/N)$, $G(q) = \eta(q)^{24}$ (with $\eta(q)$ the Dedekind function), χ_λ are the $\text{SU}(N)$ characters at level 1 and $\chi_{m, \lambda}$ are certain linear combinations thereof. $[C_i]_N$ is the reduction modulo N of the Poincaré dual of C_i , and

$$w_N(\mathcal{E}) = \sum_{i=1}^n \varepsilon_i [C_i]_N \quad [20]$$

where $\varepsilon_i = 0, 1, \dots, N-1$ are chosen independently.

Equation [19] has the expected properties under the modular group:

$$Z_\nu(\tau + 1) = e^{(i\pi/12)N(2\chi + 3\sigma)} e^{-i\pi((N-1)/N)\nu^2} Z_\nu(\tau) \\ Z_\nu(-1/\tau) = N^{-b_2/2} \left(\frac{\tau}{i} \right)^{-\chi/2} \times \sum_u e^{(2i\pi u \cdot \nu/N)} Z_u(\tau) \quad [21]$$

and also, with $Z_{\text{SU}(N)} = N^{b_1-1} Z_0$ and $Z_{\text{SU}(N)/\mathbb{Z}_N} = \sum_\nu Z_\nu$,

$$Z_{\text{SU}(N)}(-1/\tau) = N^{-\chi/2} \left(\frac{\tau}{i} \right)^{-\chi/2} Z_{\text{SU}(N)/\mathbb{Z}_N}(\tau) \quad [22]$$

which is, up to some correction factors that vanish in flat space, the original Montonen–Olive conjecture!

There is a further property to be checked which concerns the behavior of [19] under blow-ups. This property was heavily used by Vafa and Witten (1994) and demanding it in the present case was

essential in deriving the above formula. Blowing up a point on a Kähler manifold X replaces it with a new Kähler manifold \hat{X} whose second cohomology lattice is $H^2(\hat{X}, \mathbb{Z}) = H^2(X, \mathbb{Z}) \oplus I^-$, where I^- is the one-dimensional lattice spanned by the Poincaré dual of the exceptional divisor B created by the blow-up. Any allowed \mathbb{Z}_N flux $\hat{\nu}$ on \hat{X} is of the form $\hat{\nu} = \nu \oplus r$, where ν is a flux in X and $r = \lambda B$, $\lambda = 0, 1, \dots, N-1$. The main result concerning [19] is that under blowing up a point on a Kähler 4-manifold with canonical divisor as above, the partition functions for fixed 't Hooft fluxes have a factorization as

$$Z_{\hat{X}, \hat{\nu}}(\tau_0) = Z_{X, \nu}(\tau_0) \frac{\chi_\lambda(\tau_0)}{\eta(\tau_0)} \quad [23]$$

Precisely the same behavior under blow-ups of the partition function [19] has been proved for the generating function of Euler characteristics of instanton moduli spaces on Kähler manifolds. This should not come as a surprise since, as mentioned above, on certain 4-manifolds, the partition function of Vafa–Witten theory computes the Euler characteristics of instanton moduli spaces. Therefore, [19] can be seen as a prediction for the Euler numbers of instanton moduli spaces on those 4-manifolds.

Finally, the third twisted $\mathcal{N}=4$ theory also possesses two scalar supercharges, and is believed to be a certain deformation of the four-dimensional BF theory, and as such it describes essentially intersection theory on the moduli space of complexified gauge connections. In addition to this, the theory is “amphicheiral,” which means that it is invariant to a reversal of the orientation of the spacetime manifold. The terminology is borrowed from knot theory, where an oriented knot is said to be amphicheiral if, crudely speaking, it is equivalent to its mirror image. From this property, it follows that the topological invariants of the theory are completely independent of the complexified coupling constant τ .

See also: Donaldson–Witten Theory; Electric–Magnetic Duality; Hopf Algebras and q -Deformation Quantum Groups; Large- N and Topological Strings; Seiberg–Witten Theory; Topological Quantum Field Theory: Overview.

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Dynamical Systems and Thermodynamics

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Introduction

The relations between thermodynamics and dynamics are dealt with by statistical mechanics. For a given dynamical system of Hamiltonian type in a classical framework, it is usually assumed that a dynamical foundation for equilibrium statistical mechanics, namely for the use of the familiar Gibbs ensembles, is guaranteed if one can prove that the system is ergodic, that is, has no integrals of motion apart from the Hamiltonian itself. One of the main consequences is then that classical mechanics fails in explaining thermodynamics at low temperatures (e.g., the specific heats of crystals or of polyatomic molecules at low temperatures, or the black body problem), because the classical equilibrium ensembles lead to equipartition of energy for a system of weakly coupled oscillators, against Nernst's third principle. This is actually the problem that historically led to the birth of quantum mechanics, equipartition being replaced by Planck's law. At a given temperature T , the mean energy of an oscillator of angular frequency ω is not $k_B T$ (k_B being the Boltzmann constant), and thus is not independent of frequency (equipartition), but

decreases to zero exponentially fast as frequency increases.

Thus, the problem of a dynamical foundation for classical statistical mechanics would be reduced to ascertaining whether the Hamiltonian systems of physical interest are ergodic or not. It is just in this spirit that many mathematical works were recently addressed at proving ergodicity for systems of hard spheres, or more generally for systems which are expected to be not only ergodic but even hyperbolic. However, a new perspective was opened in the year 1955, with the celebrated paper of Fermi, Pasta, and Ulam (FPU), which constituted the last scientific work of Fermi.

The FPU paper was concerned with numerical computations on a system of N (actually, 32 or 64) equal particles on a line, each interacting with the two adjacent ones through nonlinear springs, certain boundary conditions having been assigned (fixed ends). The model mimics a one-dimensional crystal (or also a string), and can be described in the familiar way as a perturbation of a system of N normal modes, which diagonalize the corresponding linearized system. The initial conditions corresponded to the excitation of only a few low-frequency modes, and it was expected that energy would rather quickly flow to the high-frequency modes, thus establishing equipartition of energy, in agreement with the predictions of classical equilibrium statistical mechanics. But this did not occur within the available computation times, and the

energy rather appeared to remain confined within a packet of low-frequency modes having a certain width, as if being in a state of apparent equilibrium of a nonstandard type. This fact can be called “the FPU paradox.” In the words of Ulam, written as a comment in *Fermi’s Collected Papers*, this is described as follows: “The results of the computations were interesting and quite surprising to Fermi. He expressed the opinion that they really constituted a little discovery in providing intimations that the prevalent beliefs in the universality of mixing and thermalization in nonlinear systems may not be always justified.”

The FPU paper immediately had a very strong impact on the theory of dynamical systems, because it motivated all the modern theory of infinite-dimensional integrable systems and solitons (KdV equation), starting from the works of Zabusky and Kruskal (1965). But in this way the FPU paradox was somehow enhanced, because the FPU system turned out to be associated to the class of integrable systems, namely the systems having a number of integrals of motion equal to the number of degrees of freedom, which are in a sense the most antithermodynamic systems. The merit of establishing a bridge towards ergodicity goes to Izrailev and Chirikov (1966). Making reference to the most advanced results then available in the perturbation theory for nearly integrable systems (KAM theory), these authors pointed out that ergodicity, and thus equipartition, would be recovered if one took initial data with a sufficiently large energy. And this was actually found to be the case. Moreover, it turned out that their work, and its subsequent completion by Shepelyanski, was often interpreted as supporting the conjecture that the FPU paradox would disappear in the thermodynamic limit (infinitely many particles, with finite density and energy density). The opposite conjecture was advanced in the year 1970 by Bocchieri, Scotti, Bearzi, and Loinger, and its relevance for the relations between classical and quantum mechanics was immediately pointed out by Cercignani, Galgani, and Scotti. A long debate then followed. Possibly, some misunderstandings occurred, because in the discussions concerning the dynamical aspects of the problem reference was generally made to notions involving infinite times. In fact, it had not yet been conceived that the FPU equilibrium might actually be an apparent one, corresponding to some type of intermediate metaequilibrium state. This was for the first time suggested by researchers in Parisi’s group in the year 1982. The analogy of such a situation with that occurring in glasses was pointed out more recently.

In the present article, the state of the art of the FPU problem is discussed. The thesis of the present authors is that the FPU phenomenon survives in the thermodynamic limit, in the last mentioned sense, namely that at sufficiently low temperatures there exists a kind of metaequilibrium state surviving for extremely long times. The corresponding thermodynamics turns out to be different from the standard one predicted by the equilibrium ensembles, inasmuch as it presents qualitatively some quantum-like features (typically, specific heats in agreement with Nernst’s third principle). The key point, with respect to equilibrium statistical mechanics, is that the internal thermodynamic energy should be identified not with the whole mechanical energy, but only with a suitable fraction of it, to be identified through its dynamical properties, as was suggested more than a century ago by Boltzmann himself, and later by Nernst.

Here, it is first discussed why nearly integrable systems can be expected to present the FPU phenomenon. Then the latter is illustrated. Finally, some hints are given for the corresponding thermodynamics.

Nearly Integrable versus Hyperbolic Systems, and the Question of the Rates of Thermalization

As mentioned above, it is usually assumed that the problem of providing a dynamical foundation to classical statistical mechanics is reduced to the mathematical problem of ascertaining whether the Hamiltonian systems of physical interest are ergodic or not. However, there remains open a subtler problem. Indeed, the notion of ergodicity involves the limit of an infinite time (time averages should converge to ensemble averages as $t \rightarrow \infty$), while intermediate times might be relevant. In this connection it is convenient to distinguish between two classes of dynamical systems, namely the hyperbolic and the nearly integrable ones.

The first class, in a sense the prototype of chaotic systems, should include the systems of hard spheres (extensively studied after the classical works of Sinai), or more generally the systems of mass points with mutual repulsive interactions. For such systems it can be expected that the time averages of the relevant dynamical quantities in an extremely short time converge to the corresponding ensemble averages, so that the classical equilibrium ensembles could be safely used.

A completely different situation occurs for the dynamical systems such as the FPU systems, which are nearly integrable, that is, are perturbations of

systems having a number of integrals of motion equal to the number of degrees of freedom. Indeed, in such a case ergodicity means that the addition of an interaction, no matter how small, makes an integrable system lose all of its integrals of motion, apart from the Hamiltonian itself. And, in fact, this quite remarkable property was already proved to be generic by Poincaré, through a set of considerations which had a fundamental impact on the theory of dynamical systems itself. In view of its importance for the foundations of statistical mechanics, the proof given by Poincaré was reconsidered by Fermi, who added a subtle contribution concerning the role of single invariant surfaces. It is just to such a paper that Ulam makes reference in his comment to the FPU work mentioned above, when he says: "Fermi's earlier interest in the ergodic theory is one motive" for the FPU work.

The point is that the picture which looks at the ergodicity induced on an integrable system by the addition of a perturbation, no matter how small, somehow lacks continuity. One might expect that, in situations in which the nonlinear interaction which destroys the integrals of motion is very small (i.e., at low temperatures), the underlying integrable structure should somehow be still appreciable, in some continuous way. In fact, continuity should be recovered by making a question of times, namely by considering the rates of thermalization (to use the very FPU phrase), or equivalently the relaxation times, namely the times needed for the time averages of the relevant dynamical quantities to converge to the corresponding ensemble averages. By continuity, one clearly expects that the relaxation times diverge as the perturbation tends to zero. But more complicated situations might occur, as, for example, the existence of two (or more) relevant timescales. The point of view that timescales of different orders of magnitude might occur in dynamical systems (with the exhibition of an interesting example) and that this might be relevant for statistical mechanics, was discussed by Poincaré himself in the year 1906. Indeed, he denotes as "first-order very large time" a time which is sufficient for a system to reach a "provisional equilibrium," whereas he denotes as "second-order very large time" a time which is necessary for the system to reach its "definitive equilibrium."

The FPU Phenomenon: Historical and Conceptual Developments

We now illustrate the FPU phenomenon, following essentially its historical development. We will make

reference to Figures 1–8, which are the results of numerical integrations of the FPU dynamical system. If x_1, \dots, x_N denote the positions of the particles (of unitary mass), or more precisely the displacements from their equilibrium positions, and p_i the corresponding momenta, the Hamiltonian is

$$H = \sum_{i=1}^N \frac{p_i^2}{2} + \sum_{i=1}^{N+1} V(r_i)$$

where $r_i = x_i - x_{i-1}$ and one has taken a potential $V(r) = r^2/2 + \alpha r^3/3 + \beta r^4/4$ depending on two positive parameters α and β . Boundary conditions with fixed ends, namely $x_0 = x_{N+1} = 0$, are considered. We recall that the angular frequencies

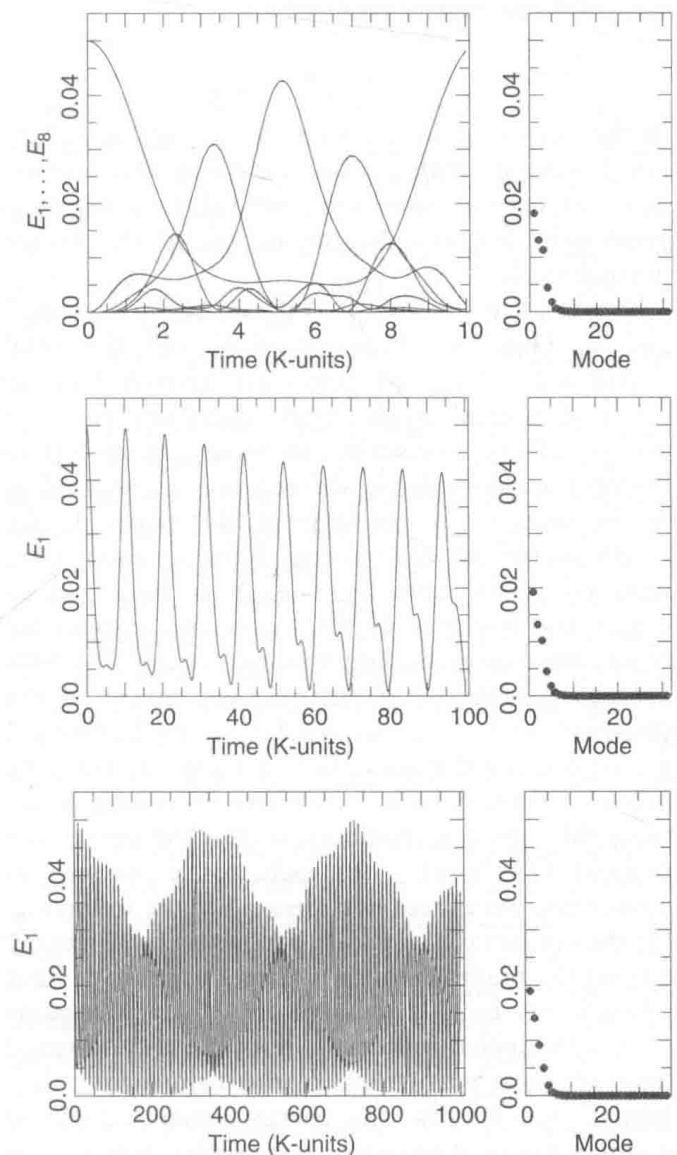


Figure 1 The FPU paradox: normal-mode energies E_j versus time (left) and energy spectrum, namely time average of E_j versus j (right) for three different timescales. The energy, initially given to the lowest-frequency mode, does not flow to the high-frequency modes within the accessible observation time. Here, $N = 32$ and $E = 0.05$.

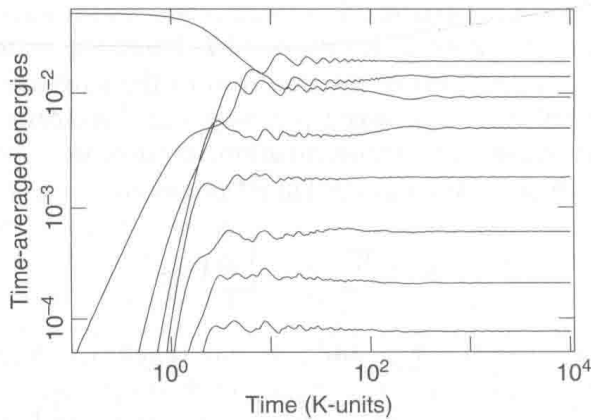


Figure 2 The FPU paradox: time averages of the energies of the modes 1, 2, ..., 8 (from top to bottom) versus time for the same run as **Figure 1**. The spectrum has reached an apparent equilibrium, different from that of equipartition predicted by classical equilibrium statistical mechanics. An exponential decay of the tail is clearly exhibited.

of the corresponding normal modes are $\omega_j = 2 \sin [j\pi/2(N+1)]$, with $j=1, \dots, N$; it is thus convenient to take as time unit the value π , which is essentially, for any N , the period of the fastest normal mode.

The original FPU result is illustrated in **Figures 1** and **2**. Here $N=32$, $\alpha=\beta=1/4$, and the total energy is $E=0.05$; the energy was given initially to the first normal mode (with vanishing potential energy). Three timescales (increasing from top to bottom) are considered, the top one corresponding to the timescale of the original FPU paper. In the boxes on the left the energies $E_j(t)$ of modes j are reported versus time ($j=1, \dots, 8$ at top, $j=1$ at center and bottom). In the boxes on the right we report the corresponding spectra, namely the time average (up to the respective final times) of the energy of mode j versus j , for $1 \leq j \leq N$. In **Figure 2** we report, for the same run of **Figure 1**, the time averages of the energies of the various modes versus time; this figure corresponds to the last one of the original FPU work. The facts to be noticed in connection with these two figures are the following: (1) the spectrum (namely the distribution of energy among the modes, in time average) appears to have relaxed very quickly to some form, which remains essentially unchanged up to the maximum observed time; (2) there is no global equipartition, but only a partial one, because the energy remains confined within a group of low-frequency modes, which form a small packet of a certain definite width; and (3) the time evolutions of the mode energies appear to be of quasiperiodic type, since longer and longer quasiperiods can be observed as the total time increases.

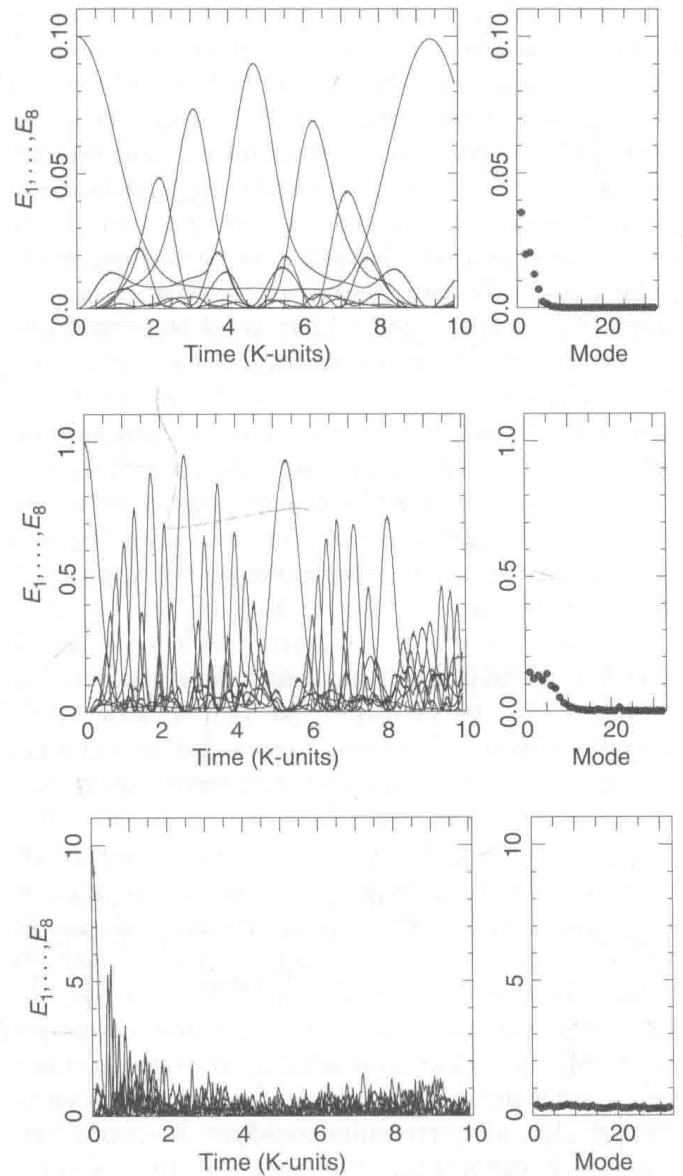


Figure 3 The Izrailev-Chirikov contribution: for a fixed observation time, equipartition is attained if the initial energy E is high enough. Here, from top to bottom, $E=0.1, 1, 10$.

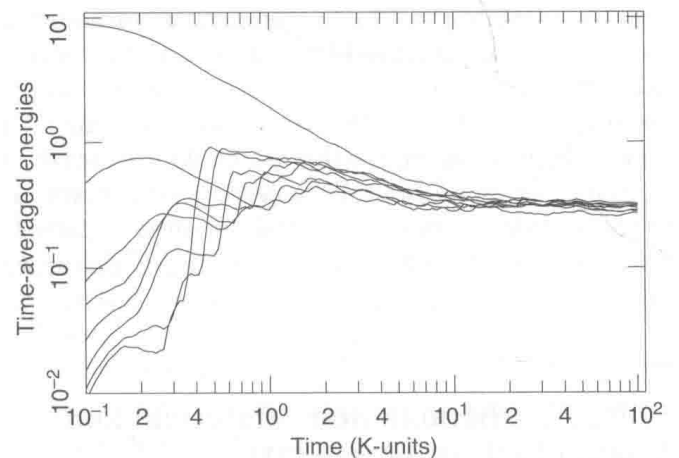


Figure 4 The Izrailev-Chirikov contribution: time averages of the mode energies versus time for the same run as at bottom of **Figure 3**.

After the works of Zabusky and Kruskal, by which the FPU system was somehow assimilated to an integrable system, the bridge toward ergodicity was made by Izrailev and Chirikov (1966), through the idea that there should exist a stochasticity threshold. Making reference to KAM theory, which had just been formulated in the framework of perturbation theory for nearly integrable systems, their main remark was as follows. It is known that KAM theory, which essentially guarantees a behavior similar to that of an integrable system, applies only if the perturbation is smaller than a certain threshold; on the other hand, in the FPU model the natural perturbation parameter is the energy E of the system. Thus, the FPU phenomenon can be expected to disappear above a certain threshold energy E_c . This is indeed the case, as illustrated in Figures 3 and 4. The parameters α, β and the class of initial data are as in Figure 1. In Figure 3 the total time is kept fixed (at 10 000 units), whereas the energy E is increased in passing from top to bottom, actually from $E=0.1$ to $E=1$ and $E=10$. One sees that at $E=10$ equipartition is attained within the given observation time; correspondingly, the motion of the modes visually appears to be nonregular. The approach to equipartition at $E=10$ is clearly exhibited in Figure 4, where the time averages of the energies are reported versus time.

There naturally arose the problem of the dependence of the threshold E_c on the number N of degrees of freedom (and also on the class of initial data). Certain semianalytical considerations of Izrailev and Chirikov were generally interpreted as suggesting that the threshold should vanish in the thermodynamic limit for initial excitations of high-frequency modes. Recently, Shepelyanski completed the analysis by showing that the threshold should vanish also for initial excitations of the low-frequency modes, as in the original FPU work (see, however, the subsequent paper by Ponno mentioned below). If this were true, the FPU phenomenon would disappear in the thermodynamic limit. In particular, the equipartition principle would be dynamically justified at all temperatures.

The opposite conjecture was advanced by Bocchieri *et al.* (1970). This was based on numerical calculations, which indicated that the energy threshold should be proportional to N , namely that the FPU phenomenon persists in the thermodynamic limit provided the specific energy $\epsilon = E/N$ is below a critical value ϵ_c , which should be definitely nonvanishing. Actually, the computations were performed on a slightly different model, in which nearby particles were interacting through a more physical Lennard-Jones potential. By taking concrete values

having a physical significance, namely the values commonly assumed for argon, for the threshold of the specific energy they found the value $\epsilon_c \simeq 0.04V_0$, where V_0 is the depth of the Lennard-Jones potential well. This corresponds to a critical temperature of the order of a few kelvin. The relevance of such a conjecture (persistence of the FPU phenomenon in the thermodynamic limit) was soon strongly emphasized by Cercignani, Galgani, and Scotti, who also tried to establish a connection between the FPU spectrum and Planck's distribution.

Up to this point, the discussion was concerned with the alternative whether the FPU system is ergodic or not, and thus reference was made to properties holding in the limit $t \rightarrow \infty$. Correspondingly, one was making reference to KAM theory, namely to the possible existence of surfaces (N -dimensional tori) which should be dynamically invariant (for all times). The first paper in which attention was drawn to the problem of estimating the relaxation times to equilibrium was by Fucito *et al.* (1982). The model considered was actually a different one (the so-called ϕ^4 model), but the results can also be extended to the FPU model. Analytical and numerical indications were given for the existence of two timescales. In a short time the system was found to relax to a state characterized by an FPU-like spectrum, with a plateau at the low frequencies, followed by an exponential tail. This, however, appeared as being a sort of metastable state. In their words: "The nonequilibrium spectrum may persist for extremely long times, and may be mistaken for a stationary state if the observation time is not sufficiently long." Indeed, on a second much larger timescale the slope of the exponential tail was found to increase logarithmically with time, with a rate which decreases to zero with the energy. This is an indication that the time for equipartition should increase as an exponential with the inverse of the energy.

This is indeed the picture that the present authors consider to be essentially correct, being supported by very recent numerical computations, and by analytical considerations. Curiously enough, however, such a picture was not fully appreciated until quite recently. Possibly, the reason is that the scientific community had to wait until becoming acquainted with two relevant aspects of the theory of dynamical systems, namely Nekhoroshev theory and the relations between KdV equation and resonant normal-form theory.

The first step was the passage from KAM theory to Nekhoroshev theory. Let us recall that, whereas in KAM theory one looks for surfaces which are invariant (for all times), in Nekhoroshev theory one

looks instead for a kind of weak stability involving finite times, albeit “extremely long” ones, as they are found to increase as stretched exponentials with the inverse of the perturbative parameter. Thus, one meets with situations in which one can have instability over infinite times, while having a kind of practical stability up to exponentially long times. Notice that Nekhoroshev’s theory was formulated only in the year 1974, and that it started to be known in the West only in the early 1980s, just because of its interest for the FPU problem. Another interesting point is that just in those years one started to become acquainted with a related historical fact. Indeed, the idea that equipartition might require extremely long times, so that one would be confronted with situations of a practical lack of equipartition, has in fact a long tradition in statistical mechanics, going back to Boltzmann and Jeans, and later (in connection with sound dispersion in gases of polyatomic molecules) to Landau and Teller.

In this way the idea of the existence of extremely long relaxation times to equipartition came to be accepted. The ingredient that was still lacking is the idea of a quick relaxation to a metastable state. The importance of this should not be overlooked. Indeed, without it one cannot at all have a thermodynamics different from the standard equilibrium one corresponding to equipartition. This was repeatedly emphasized, against Jeans, by Poincaré on general grounds and by Nernst on empirical grounds. The full appreciation of this latter ingredient was obtained quite recently (although it had been clearly stated by Fucito *et al.* (1982)). A first hint in this direction came from the realization (see Figure 5) of a deep analogy between the FPU phenomenon and the phenomenology of glasses. Then there came a strong numerical indication by Berchialla, Galgani, and Giorgilli. Finally, from the analytical point of view, there was a suitable revisitation (by Ponno) of the traditional connection between the FPU system and the KdV equation with its solitons. The relevant points are the following: (1) the KdV equation describes well the solutions of the FPU problem (for initial data of FPU type) only on a “short” timescale, which increases as a power of $1/\epsilon$, and so describes only a first process of quick relaxation; (2) the corresponding spectrum has a very definite analytical form, the energy being spread up to a maximal frequency $\bar{\omega}(\epsilon) \simeq \epsilon^{1/4}$ and then decaying exponentially; and (3) the relevant formulas contain the energy only through the specific energy ϵ , and thus can be expected to hold also in the thermodynamic limit. It should be mentioned, however, that all the results of an

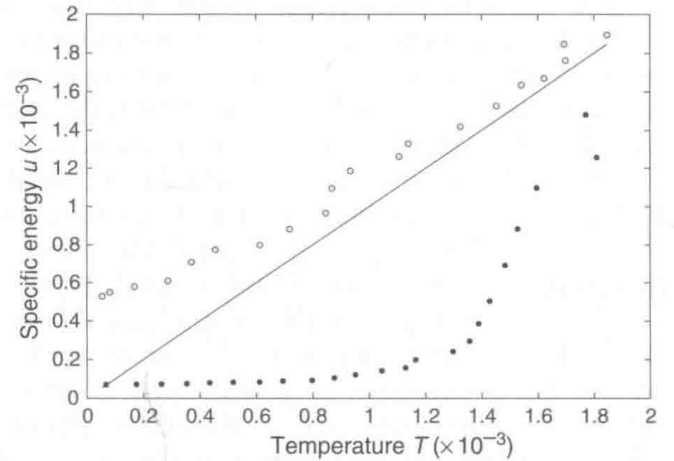


Figure 5 Analogy with glasses: the specific energy u of an FPU system is plotted versus temperature T for a cooling process (upper curve) and a heating process (lower curve). The FPU system is kept in contact with a heat reservoir, whose temperature is changed at a given rate. At low temperatures the system does not have time to reach the equilibrium curve $u = T$ (with $k_B = 1$).

analytic type mentioned above have a purely formal character, because up to now none of them was proved, in the thermodynamic limit, in the sense of rigorous perturbation theory. This requires a suitable readaptation of the known techniques, which is currently being obtained both in connection with Nekhoroshev’s theorem (in order to explain the extreme slowness of a possible final approach to equilibrium) and in connection with the normal-form theory for partial differential equations (in order to explain the fast relaxation to the metaequilibrium state).

In conclusion, for the case of initial conditions of the FPU type (excitation of a few low-frequency modes) the situation seems to be as follows. The first phenomenon that occurs in a “short” time (of the order of $(1/\epsilon)^{3/4}$) is a quick relaxation to the formation of what can be called a “natural packet” of low-frequency modes extending up to a certain maximal frequency $\bar{\omega} \simeq \epsilon^{1/4}$. This is a phenomenon which has nothing to do with any diffusion in phase space. In fact, it shows up also for an integrable system such as a Toda lattice (as will be illustrated below), and should be described by a suitable resonant normal form related to the KdV equation. One has then to take into account the fact that the domain of the frequencies in the FPU model is bounded ($\omega < 2$ in the chosen units). Now, as the function $\bar{\omega}(\epsilon)$ is monotonic, this fact leads to the existence of a critical value ϵ_c of the specific energy ϵ , defined by $\bar{\omega}(\epsilon_c) = 2$. Indeed, for $\epsilon > \epsilon_c$ the quick relaxation process leads altogether to equipartition. Below the threshold, instead, the same quick process leads to the formation of an FPU-like spectrum,

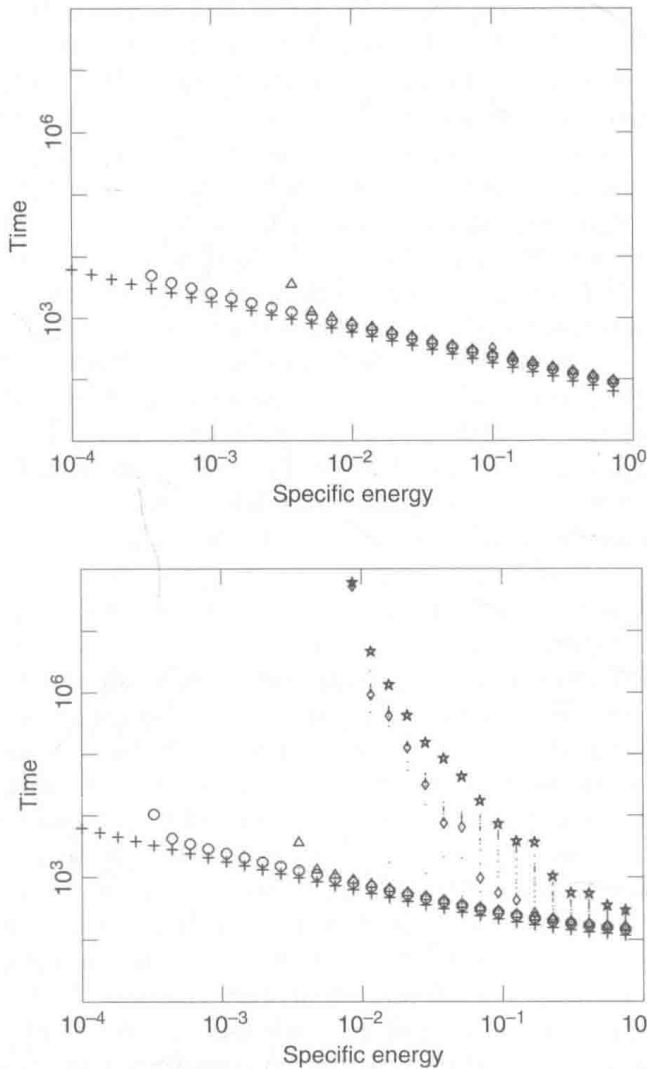


Figure 6 Time needed to form a packet versus specific energy for the FPU model (bottom) and the corresponding Toda model (top). Different symbols refer to packets of different width. The existence of two timescales below a critical specific energy in the FPU model is exhibited.

involving only modes of sufficiently low frequency. This should, however, be a metastable state (which might be mistaken for a stationary one), which should be followed, on a second timescale, by a relaxation to the final equilibrium, through a sort of Arnol'd diffusion requiring extremely long Nekhoroshev-like times. This is actually the way in which the old idea of a threshold, originally conceived in terms of KAM tori, is now recovered even for ergodic systems, in terms of timescales.

The existence of a process of quick relaxation, and of a threshold in the above-mentioned sense, is illustrated in Figures 6 and 7. In Figure 6 the lower part refers to the FPU model, while the upper one refers to a corresponding Toda model. The latter is in a sense the prototype of an integrable nonlinear system; with respect to the FPU case, the difference is that the potential $V(r)$ is now exponential. The

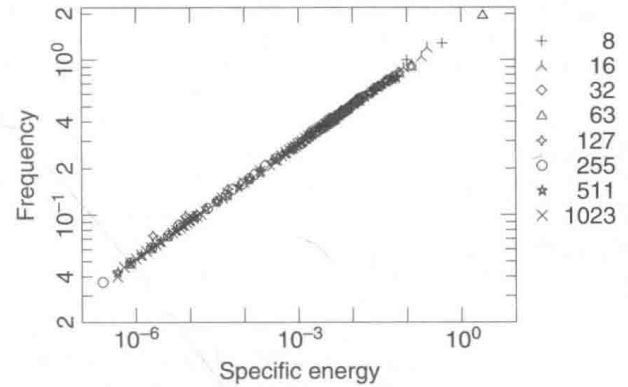


Figure 7 Width of the natural packet versus specific energy, for N ranging from 8 to 1023. Reproduced from Berchiulla L, Galgani L, and Giorgilli A (2004) Localization of energy in FPU chains, *Discr. Cont. Dyn. Systems B* 11: 855–866, with permission from American Institute of Mathematical Sciences.

parameters of the exponential were chosen so that the two models coincide up to cubic terms in the potential. With the energy given to the lowest-frequency mode, the figure shows the time needed in order that energy spreads up to a mode \bar{k} , for several values of \bar{k} , as a function of ϵ . It is seen that in the Toda model (top) there is formed a packet extending up to rather well-defined width, and that this occurs within a relaxation time increasing as a power of $1/\epsilon$. An analogous phenomenon occurs for the FPU model (bottom). The only difference is that, below a critical specific energy $\epsilon_c \simeq 0.1$, there exists a subsequent relaxation time to equipartition, which involves a time growing faster than any inverse power of ϵ . Such a second phenomenon is due to the nonintegrable character of the FPU model. In Figure 7 the width of the natural packet for the FPU model is exhibited, by reporting the frequency $\bar{\omega}$ of its highest mode as a function of ϵ . As one sees, the numerical results clearly indicate the existence of a relation $\bar{\omega} \simeq \epsilon^{1/4}$, which holds for a number of degrees of freedom N ranging from 8 to 1023. This is actually the law which is predicted by resonant normal-form theory.

Boltzmann and Nernst Revisited

All the results illustrated above refer to initial data of FPU type, namely with an excitation of a few low-frequency modes. However, from the point of view of statistical mechanics, such initial data are exceptional, and one should rather consider initial data extracted from the Gibbs distribution at a certain temperature. One can then couple the FPU system to a heat bath at a slightly different temperature, and look at the spectrum of the FPU system after a certain time. The result, for the case of a heat bath at a higher temperature, is shown in

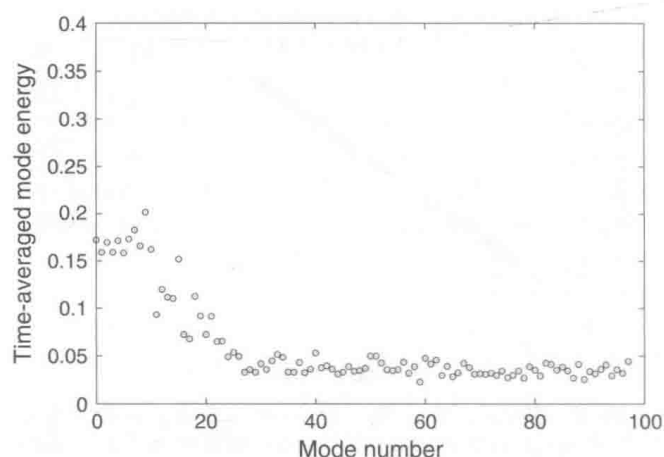


Figure 8 A case of an FPU system initially at equilibrium and thus in equipartition. Spectrum of the FPU system after it was kept in contact with a heat reservoir at a higher temperature.

Figure 8. Clearly, here one has a situation similar to that occurring for initial data of FPU type, because only a packet of low-frequency modes exhibits a reaction, each of its modes actually adapting itself to the temperature of the bath, whereas the high-frequency modes do not react at all, that is, remain essentially frozen.

This capability of reacting to external disturbances (which seems to pertain only to a fraction of the mechanical energy initially inserted into the system) can be characterized in a quantitative way through an estimate of the fluctuations of the total energy of the FPU system. This is indeed the sense of the fluctuation-dissipation theorem, the precursor of which is perhaps the contribution of Einstein to the first Solvay conference (1911). Through such a method, the specific heat of the FPU system is estimated (apart from a numerical factor) by the time average of $[E(t) - E(0)]^2$, where $E(t)$ is the energy, at time t , of the FPU system in dynamical contact with a heat bath (at the same temperature from which the initial data are extracted). Usually, in the spirit of ergodic theory, one looks at the infinite-time limit of such a quantity. But in the spirit of the metastable picture described above, one can check whether the time average presents a previous stabilization to some value smaller than the one predicted at equilibrium. Such a result, which is in qualitative agreement with the third principle, has indeed been obtained (by Carati and Galgani) recently.

In conclusion, in situations of metaequilibrium such as those existing in the FPU model at low temperatures, a thermodynamics can still be formulated. Indeed, by virtue of the quick relaxation process described above, the time averages of the relevant quantities are found to stabilize in rather short times. In this way, one overcomes the critique of Poincaré to Jeans, namely that one cannot have a thermodynamics at all if reference is made only to the existence of

extremely long relaxation times to the final equilibrium. A relaxation to a “provisional equilibrium” within a “first-order very large time” (to quote Poincaré) is required. The difference with respect to the standard equilibrium thermodynamics relies now in the mechanical interpretation of the first principle. Indeed, the internal thermodynamic energy is identified not with the whole mechanical energy, but just with that fraction of it which is capable of reacting in short times to the external perturbations.

This is the way in which the old idea of Boltzmann (and Jeans) might perhaps be presently implemented. For what concerns the fraction of the mechanical energy which is not included in the thermodynamic internal energy, as not being able to react in relatively short times, this should somehow play the role of a zero-point energy. This was suggested in the year 1971 by C Cercignani. But in fact, such a concept was put forward by Nernst himself in an extremely speculative work in 1916, where he also advanced the concept that, for a system of oscillators of a given frequency, there should exist both dynamically ordered (*geordnete*) and dynamically chaotic (*ungeordnete*) motions, the latter being prevalent above a certain energy threshold. According to him, this fact should be relevant for a dynamical understanding of the third principle and of Planck’s law.

It is well known that the modern theory of dynamical systems has led to familiarity with the (sometimes abused) notions of order and chaos and of a transition between them. One might say that the FPU work just forced the scientific community to take into account such notions in connection with the principle of equipartition of energy. It is really fascinating to see that the same notions, with the same terminology, had already been introduced much earlier on purely thermodynamic grounds, in connection with the relations between classical and quantum mechanics.

See also: Boundary Control Method and Inverse Problems of Wave Propagation; Central Manifolds, Normal Forms; Ergodic Theory; Fourier Law; Gravitational N -body Problem (Classical); Newtonian Fluids and Thermohydraulics; Nonequilibrium Statistical Mechanics: Interaction between Theory and Numerical Simulations; Quantum Statistical Mechanics: Overview; Regularization for Dynamical Zeta Functions; Stability Theory and KAM; Toda Lattices; Weakly Coupled Oscillators.

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Dynamical Systems in Mathematical Physics: An Illustration from Water Waves

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Introduction

The purpose of this article is to describe some basic problems related to the interplay between dynamical systems and mathematical physics. Since it is impossible to be exhaustive in these topics, the focus here is on water-wave models. These mathematical models are described by partial differential equations that can be understood as dynamical systems in a suitable infinite-dimensional phase space.

We will not address the original equations for two-dimensional (2D) surface water waves, even if we know that dynamical-system methods can help to exhibit some solitary waves for the equations. The reader is referred to relevant articles in this encyclopedia for details. Another approach is to seek these 2D surface water waves as saddle points for some Hamiltonians, which too is discussed elsewhere in this work.

This article presents these arguments on some asymptotical models for the propagation of surface water waves.

Asymptotical Models in Hydrodynamics

To begin with, consider an irrotational fluid in a canal that is governed by the Euler equations and

that is subject to gravitational forces. For a canal of finite depth, Boussinesq (1877) and Korteweg–de Vries (KdV) (1890) obtained the following model for unidirectional long waves:

$$u_t + u_x + u_{xxx} + uu_x = 0 \quad [1]$$

Sometimes we drop the u_x term on the left-hand side of [1], thanks to a suitable change of coordinates. Alternatively, we can also deal with the so-called generalized KdV equation, which reads

$$u_t + u_{xxx} + u^k u_x = 0 \quad [2]$$

where k is a positive integer. There are also other models designed to represent long waves in shallow water. Let us introduce the regularized long-wave equation (also referred to as the Benjamin–Bona–Mahony equation) that reads

$$u_t - u_{txx} + u_x + uu_x = 0 \quad [3]$$

or the Camassa–Holm equation

$$u_t - u_{txx} + 3uu_x = 2u_x u_{xx} + uu_{xxx} \quad [4]$$

For deep water, a well-known model was introduced by Zakharov (1968)

$$iu_t + u_{xx} + \varepsilon |u|^2 u = 0 \quad [5]$$

which describes the slow modulations of wave packets. Here the unknown $u(x, t)$ takes values in \mathbb{C} , and this nonlinear Schrödinger equation is in fact a system. In these equations, ε is either 1 or -1 ; throughout this article, we shall refer to the former case as the focusing case and to the latter

as the defocusing case. We may also substitute $|u|^{2p}u$ in the nonlinear term in [5] to obtain alternate models.

The variable t represents the time and the space variable x belongs either to \mathbb{R} or to a finite interval when we are dealing with periodic flows.

The above models are intended to describe the propagation of unidirectional waves. For two-way waves, see Bona *et al.* (2002).

Actually, these equations feature particular solutions, the so-called traveling waves. Let us recall, for instance, that for generalized KdV equation [2] these solutions are

$$u(t, x) = Q_c(x - ct) \quad [6]$$

$$Q_c(x) = c^{1/p} Q(\sqrt{c}x) \quad [7]$$

$$Q(x) = (3 \operatorname{ch}^{-2}(px))^{1/p} \quad [8]$$

These so-called solitons (Figure 1) move to the right without changing their shape; c is the speed of propagation. In real life, this phenomenon was observed by Russel (1834). Riding his horse, he was able to follow for miles the propagation of such a wave on the canal from Edinburgh to Glasgow. On the other hand, Camassa–Holm equations are designed to describe the propagation of peaked solitons as shown in Figure 2.

Focusing nonlinear Schrödinger equations also feature solitary waves that read $u_\omega(t, x) = \exp(i\omega t)Q(x)$, where Q is solution to

$$Q_{xx} - \omega Q + Q^{2p+1} = 0 \quad [9]$$

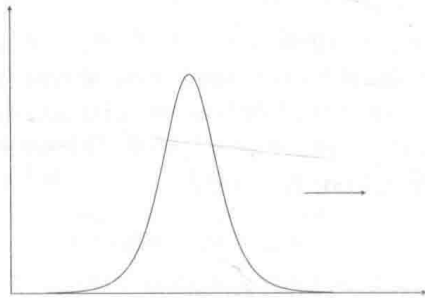


Figure 1 A soliton.

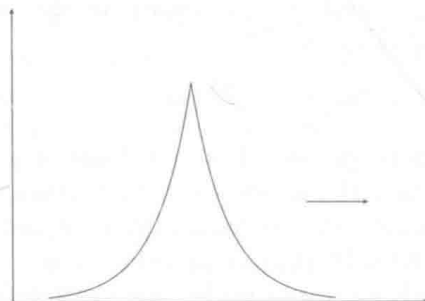


Figure 2 Peaked soliton.

There are numerous examples of equations or systems of equations that model 2D surface water waves. Among all these models, a first issue is to identify the relevant models insofar as the dynamical properties are concerned. Indeed, we address here the question of stability of solitary waves (up to the symmetries of the equation). For instance, the orbital stability for cubic Schrödinger reads: for any $\varepsilon > 0$, there exists a neighborhood Ω of $u_\omega(x, 0)$ such that any trajectory starting from Ω satisfies

$$\sup_t \inf_\theta \inf_y \|u(t) - \exp(i\theta)u_\omega(t, \cdot - y)\|_{H^1} \leq \varepsilon \quad [10]$$

Another issue consists in the interaction of N solitons. Schneider and Wayne (2000) have addressed the issue of the validity of water-wave models when this interaction is concerned.

Assume now that the validity of these models is granted. To consider [1] or [5] as a dynamical system, the next issue is then to consider the initial-value problem.

The Initial-Value Problem

Let us supplement these equations with initial data u_0 in some Sobolev space. We shall consider either

$$H^s(\mathbb{R}) = \left\{ u; \int_{\mathbb{R}} (1 + |\xi|^2)^s |\hat{u}(\xi)|^2 d\xi < +\infty \right\} \quad [11]$$

in the case where x belongs to the whole line, or the corresponding Sobolev space with periodic boundary conditions. It should be examined whether these equations provide a continuous flow $S(t): u_0 \rightarrow u(t)$ in these functional spaces (at least locally in time). We would like to point out that for each Sobolev space under consideration, we may have a different flow. This fact is at the heart of infinite-dimensional dynamical systems.

The initial-value problem was a challenge for decades for low norms, that is for small s . The last breakthrough was performed by Bourgain (1993). Let us present the method for KdV equation. Consider $U(t)u_0$ the solution of the Airy equation

$$u_t + u_{xxx} = 0, \quad u(0) = u_0 \quad [12]$$

Without going into further details, the idea is to perform a fixed-point argument to the Duhamel's form of the equation,

$$u(t) = U(t)u_0 - \frac{1}{2} \int_0^t U(t-s) \partial_x(u^2(s)) ds \quad [13]$$

in a suitable mixed-spacetime Banach space whose norm reads $\|U(-t)u(t, x)\|_{H_t^b H_x^s}$. This relies on fine properties in harmonic analysis. Thanks to this method, we know that the Schrödinger equation [5] and the KdV equation [1] are well-posed in, respectively, $H^s(\mathbb{R}), s \geq 0$ and $H^s(\mathbb{R}), s > -3/4$, locally in time. For the periodic case, the results are slightly different. We would like to point out that both KdV and nonlinear Schrödinger equations provide semigroups $S(t)$ that do not feature smoothing effect. A trajectory that starts from H^s remains in H^s ; indeed, we can also solve these partial differential equations backward in time.

The next issue is to determine if these flows are defined for all times. Loosely speaking, the following alternative holds true: either the local flow in H^s extends to a global one, or some blow-up phenomenon occurs, that is, $\|S(t)u_0\|_{H^s}$ collapses in finite time.

To this end, let us observe that, for instance, the mass $\int_{\mathbb{R}} |u(x)|^2 dx$ is conserved for both KdV and nonlinear Schrödinger flows. Therefore, one can prove that the solutions in L^2 are global in time. It is worthwhile to observe that the Bourgain method also provides some global existence results below the energy norm.

Consider now the flow of the solutions in H^1 . The second invariant for nonlinear Schrödinger equations reads

$$\int_{\mathbb{R}} |u_x(x)|^2 dx - \frac{\varepsilon}{p+1} |u(x)|^{2p+2} dx \quad [14]$$

Therefore, the local solutions in H^1 extend to global ones in the defocusing case ($\varepsilon = -1$). In the focusing case, the situation is more contrasted. The solution is global if the nonlinearity is less than an H^1 -critical value ($p=2$ for Schrödinger, and $k=4$ for generalized KdV equation). This critical value depends on some Sobolev embeddings as

$$\int_{\mathbb{R}} |u(x)|^{2p+2} dx \leq C_p \|u\|_{L^2}^{p+1} \|u_x\|_{L^2}^p \quad [15]$$

Therefore, since the mass is constant, the second invariant controls the H^1 norm of the solution if $p < 2$. Note that the critical power of the nonlinearity depends also on the dimension of the space; it is the cubic Schrödinger that is critical in $H^1(\mathbb{R}^2)$. It is well known that, for some initial data, blow-up phenomena can occur for 2D cubic Schrödinger equations. Moreover, the behavior of blow-up solutions is more or less understood. This analysis was performed using the conformal invariance of the equation. For quintic Schrödinger equation,

which is critical in 1D, this conformal invariance states that if $u(t, x)$ is solution, then

$$v(t, x) = |t|^{-1/2} \exp\left(\frac{ix^2}{4t}\right) \bar{u}\left(\frac{1}{t}, \frac{x}{t}\right) \quad [16]$$

is also solution.

On the other hand, for the generalized KdV equation, there is no conformal invariance and the blow-up issue had been open for years. There was some numerical evidence that blow-up can occur for $k=4$. Recently, Martel and Merle (2002) have given a complete description of the blow-up profile for this equation. Their methods are quite complex and rely on an ejection of mass at infinity in a suitable coordinate system.

In the discussion so far we have presented some quantities that are invariant by the flow of the solutions. This is related to the Hamiltonian structure of the dynamical systems under consideration.

Hamiltonian Systems in Hydrodynamics

The study of Hamiltonian systems has developed beyond celestial mechanics (the famous n -body problems) to other fields in mathematical physics. We focus here on dynamical systems that read

$$u_t = J \frac{\partial}{\partial u} H(u) \quad [17]$$

where H is the Hamiltonian and J some skew-symmetric operator. For instance, [1] is a Hamiltonian system with $J = \partial_x$ (i.e., an unbounded skew-symmetric operator) and

$$H(u) = \frac{1}{2} \int (u^2 - u_x^2) dx + \frac{1}{6} \int u^3 dx \quad [18]$$

There is a subclass of Hamiltonian systems that are integrable by inverse-scattering methods. For instance, [1] belongs to this class. Indeed, these methods give a complete description of the asymptotics when $t \rightarrow \pm\infty$. It is well known (Deift and Zhou 1993) that, asymptotically, any solution to KdV equation consists of a wave train moving to the right in the physical space up to a dispersive part moving to the left.

On the other hand, a generic Hamiltonian system is not integrable. The study of the asymptotics and of the dynamical properties of such a system deserves another analysis. We say that a system features asymptotic completeness if there exist u_+

and u_- such that the solution $u(t)$ of [17] supplemented with initial data u_0 satisfies

$$\|u(t) - U(t)u_+\| \rightarrow 0 \quad [19]$$

$$\|u(t) - U(t)u_-\| \rightarrow 0 \quad [20]$$

when, respectively, $t \rightarrow +\infty$ or $t \rightarrow -\infty$. Here $U(t)u_0$ is the solution of the free equation, that is, the associated linear equation, supplemented with initial data u_0 ; for instance, the Airy equation is the free equation related to the KdV equation. The operators $u_- \rightarrow u_0 \rightarrow u_+$ are called wave operators. This is related to the Bohr's transition in quantum mechanics. Loosely speaking, we are able to prove these scattering properties for high powers in the nonlinearity for subcritical defocusing Schrödinger equations.

The asymptotics of trajectories can be more complicated. Let us recall that the stability of traveling waves is also an important issue in understanding the dynamical properties of these models. For instance, let us point out that Martel and Merle proved the asymptotic stability of the sum of N solitons for KdV in the subcritical case.

Beyond these asymptotics we are interested in the case where the permanent regime is chaotic (or turbulent). A scenario is that there exist quasiperiodic solutions of arbitrarily order N for the system under consideration. The next challenge about these Hamiltonian systems is to apply the Kolmogorov–Arnol'd–Moser theory to exhibit this type of solutions to systems like [17]. Here we restrict our discussion to the case of bounded domains, with either periodic or homogeneous Dirichlet conditions. Then, let us introduce the following definition: a solution is quasiperiodic if there exist a finite number N of frequencies ω_k such that

$$u(t, x) = \sum_{l=1}^N u_l(x) \exp(i\omega_k t) \quad [21]$$

This extends the case of periodic solutions ($N=1$), which are isomorphic to the torus. To prove the existence of such structures, one idea is then to imbed N -dimensional invariant tori into the phase space of solutions. One may approximate the infinite-dimensional Hamiltonian by a sequence of finite ones and consider the convergence of iterated symplectic transformations, or one solves directly some nonlinear functional equation. Actually, the difficulty is that resonances can occur. Resonances occur when there are some linear combinations of the frequencies that vanish (or that are arbitrarily close to 0). This introduces a small divisor problem

in a phase space that has infinite dimension. To overcome these difficulties, a Nash–Moser scheme can be implemented (Craig 1996). There are numerous such open problems. For instance, let us observe that known results are essentially only for the case where the dimension of the ambient space is 1. On the other hand, quasiperiodic solutions correspond to N -dimensional invariant tori for the flow of solutions; one may seek for Lagrangian invariant tori that correspond to the case where $N = +\infty$. Current research is directed towards extending this analysis.

Another issue is to seek invariant measures for these Hamiltonian dynamical systems, as in statistical mechanics. Bourgain was successful in performing this analysis for some nonlinear Schrödinger equations either in the case of periodic boundary conditions or in the whole space. This result is an important step in the ergodic analysis of our Hamiltonian dynamical systems. This could explain the Poincaré recurrence phenomena observed numerically for these types of equations: some particular solutions seem to come back to their initial state after a transient time. This point will not be developed here.

All these results are properties of conservative dynamical systems. We now address the case when some dissipation takes place.

Dissipative Water-Wave Models

To model the effect of viscosity on 2D surface water waves, we go back to a flow governed by the Navier–Stokes equations and we proceed to obtain damped equations (Ott and Sudan 1970, Kakutani and Matsuuchi 1975). In fact, the damping in KdV equations can be either a diffusion term that leads to study the equation

$$u_t + u_{xxx} + uu_x = \nu u_{xx} \quad [22]$$

where ν is a positive number analogous to the viscosity, or a zero-order term $-\nu u$ on the right-hand side of [22]. In the first case, we obtain a KdV–Burgers equation that has some smoothing effect in time. In the second case, we have a zero-order dissipation term. A nonlocal term would be $\nu \mathcal{F}^{-1}(|\xi|^{2\beta} \hat{u}(\xi))$ for $\beta \in [0, 1]$, where $\mathcal{F}(u) = \hat{u}$ denotes the Fourier transform of u .

A first issue concerning damped water-wave equations is to estimate the decay rate of the solutions towards the equilibrium (no decay) when $t \rightarrow +\infty$. For [22] the ultimate result is that, for initial data $u_0 \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})$, the L^2 norm of the solution decays like $t^{-1/4}$ (Amick *et al.* 1989). Energy methods have been developed to handle these problems, as the Shonbeck's splitting method.

The center manifold theory is another approach that is employed in dynamical systems. The aim is to prove the existence of a finite-dimensional manifold that is invariant (in a neighborhood of the origin) by the flow of the solutions and that attracts the other trajectories with high speed. Therefore, this manifold, and the trajectories therein, monitor the decay rate of the solutions towards the origin. The construction of such a manifold relies on splitting properties of the spectrum of the associated linearized operator (Gallay and Wayne 2002). Using a suitable change of variables (that moves the continuous spectrum away from the origin), Gallay and Wayne were able to construct such a manifold in an infinite-dimensional phase space.

Another issue is the understanding of the dynamics for damped–forced water-wave equations as

$$u_t + uu_x + u_{xxx} + \nu u = f(x) \quad [23]$$

The dynamical system approach is the attractor theory (Temam 1997). Equations such as [23] provide dissipative semigroups $S(t)$ in some energy spaces. The theory has developed for years and we know that these dynamical systems feature global attractors. A global attractor is a compact subset in the energy space under consideration which is invariant by the flow of the solutions and that attracts all the trajectories when $t \rightarrow +\infty$. Moreover, if we deal with periodic boundary conditions, this global attractor has finite fractal (or Hausdorff) dimension. This dimension depends on the data concerning ν and f .

Actually, eqn [23] provides semigroups either in $L^2(\mathbb{R})$, $H^1(\mathbb{R})$, or in $H^2(\mathbb{R})$. These three dynamical systems feature global attractors $\mathcal{A}_0, \mathcal{A}_1, \mathcal{A}_2$. From the viewpoint of physics, the attractors describe the permanent regime of the flow. One may wonder if this permanent regime depends on the space chosen for the mathematical study. Eventually, the last result for this issue establish that $\mathcal{A}_0 = \mathcal{A}_1 = \mathcal{A}_2$. This property is equivalent to prove the asymptotical smoothing effect for the associated semigroup: even if $S(t)$ is not a smoothing operator for finite t , then all solutions converge to a smooth set when t goes to the infinity.

All these results are for subcritical nonlinearities. As already noted, dissipation provides smoothing at infinity. Nevertheless, damping does not prevent blow-up. Let us illuminate this by the following result due to Tsutsumi (1984). The damped Schrödinger equation

$$iu_t + i\nu u + u_{xx} + |u|^{2p}u = 0 \quad [24]$$

features blow-up solutions in $H^1(\mathbb{R})$ for $p > 2$, even if all solutions are damped in $L^2(\mathbb{R})$ with exponential speed.

This completes the discussion of damped–forced water-wave equations. We now consider equations that are forced with a random forcing term.

Stochastic Water-Wave Models

During the modeling process that led to KdV or Schrödinger equations from Euler equation, we have neglected some low-order terms. We now model these terms by a noise and we are led to a new randomly forced dynamical system that reads

$$u_t + u_x + u_{xxx} + uu_x = \gamma \dot{\xi} \quad [25]$$

Here one may assume that $\xi(x, t)$ is a Gaussian process with correlations

$$\mathbb{E}(\dot{\xi}(x, t)\dot{\xi}(y, s)) = \delta_{x-y}\delta_{t-s} \quad [26]$$

that is, a spacetime white noise. The parameter γ is the amplitude of the process. Unfortunately, due to the lack of smoothing effect of KdV or Schrödinger equations, it is more convenient to work with a noise that is correlated in space, satisfying

$$\mathbb{E}(\dot{\xi}(x, t)\dot{\xi}(y, s)) = c(x - y)\delta_{t-s} \quad [27]$$

here $c(x - y)$ is some smooth ansatz for δ_{x-y} , defined from some Hilbert–Schmidt kernel K as

$$c(x - y) = \int_{\mathbb{R}} K(x, z)K(y, z) dz$$

We also consider random perturbation of focusing Schrödinger equation, which reads either

$$u_t + iu_{xx} + i|u|^{2p}u = u\dot{\xi} \quad [28]$$

(which represents a multiplicative noise) or

$$u_t + iu_{xx} + i|u|^{2p}u = i\gamma\dot{\xi} \quad [29]$$

(which is an additive noise). In the former case, the noise acts as a potential, while in the latter case it represents a forcing term. These equations also model the propagation of waves in an inhomogeneous medium.

Research is in progress to study these stochastic dynamical systems. To begin with, the theory of the

initial-value problem has to be established in this new context (see, e.g., de Bouard and Debussche (2003)).

One challenge is to understand the effect of noise on dynamical properties of the particular solutions described above, for instance, the solitary waves for Schrödinger equation, either in the subcritical case $p < 2$ or in the critical case $p = 2$ and beyond.

Results obtained both theoretically and numerically on the influence of the noise on blow-up phenomena (random process) for generalized Schrödinger equations are likely almost-sure results.

On the one hand, if the noise is additive and the power supercritical, $p > 1$, there is some numerical evidence that a spacetime white noise can delay or even prevent the blow-up. However, if the noise is not so irregular (as for the correlated in space noise described above) it seems that any solution blows up in finite time.

de Bouard and Debussche have proved that for either an additive or a multiplicative noise, any smooth and localized (in space) initial data give rise to a trajectory that collapses in arbitrarily small time with a positive probability. This contrasts with the deterministic case, where only particular initial data could lead to blow-up trajectories. Actually, the noise enforces that any trajectory must pass through this blow-up region, with a positive probability.

Acknowledgment

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See also: Bifurcations in Fluid Dynamics; Bifurcation Theory; Breaking Water Waves; Cellular Automata; Central Manifolds, Normal Forms; Dissipative Dynamical Systems of Infinite Dimension; Fractal Dimensions in Dynamics; Hamilton–Jacobi Equations and Dynamical Systems: Variational Aspects; Metastable States; Newtonian Fluids and Thermohydraulics; Nonlinear Schrödinger Equations; Quantum Calogero–Moser Systems; Random Dynamical Systems; Scattering, Asymptotic Completeness and Bound States; Stability

Problems in Celestial Mechanics; Stochastic Resonance; Symmetry and Symplectic Reduction.

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Effective Field Theories

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Introduction

Effective field theories (EFTs) are the counterpart of the “theory of everything.” They are the field theoretical implementation of the quantum ladder: heavy degrees of freedom need not be included among the quantum fields of an EFT for a description of low-energy phenomena. For example, we do not need quantum gravity to understand the hydrogen atom nor does chemistry depend upon the structure of the electromagnetic interaction of quarks.

EFTs are approximations by their very nature. Once the relevant degrees of freedom for the problem at hand have been established, the corresponding EFT is usually treated perturbatively. It does not make much sense to search for an exact solution of the Fermi theory of weak interactions. In the same spirit, convergence of the perturbative expansion in the mathematical sense is not an issue. The asymptotic nature of the expansion becomes apparent once the accuracy is reached where effects of the underlying “fundamental” theory cannot be neglected any longer. The range of applicability of the perturbative expansion depends on the separation of energy scales that define the EFT.

EFTs pervade much of modern physics. The effective nature of the description is evident in atomic and condensed matter physics. The present article will be restricted to particle physics, where EFTs have become important tools during the last 25 years.

Classification of EFTs

A first classification of EFTs is based on the structure of the transition from the “fundamental” (energies $> \Lambda$) to the “effective” level (energies $< \Lambda$).

1. *Complete decoupling* The fundamental theory contains heavy and light degrees of freedom.

Under very general conditions (decoupling theorem, Appelquist and Carazzone 1975) the effective Lagrangian for energies $\ll \Lambda$, depending only on light fields, takes the form

$$\mathcal{L}_{\text{eff}} = \mathcal{L}_{d \leq 4} + \sum_{d > 4} \frac{1}{\Lambda^{d-4}} \sum_{i_d} g_{i_d} O_{i_d} \quad [1]$$

The heavy fields with masses $> \Lambda$ have been “integrated out” completely. $\mathcal{L}_{d \leq 4}$ contains the potentially renormalizable terms with operator dimension $d \leq 4$ (in natural mass units where Bose and Fermi fields have $d = 1$ and $3/2$, respectively), the g_{i_d} are coupling constants and the O_{i_d} are monomials in the light fields with operator dimension d . In a slightly misleading notation, $\mathcal{L}_{d \leq 4}$ consists of relevant and marginal operators, whereas the O_{i_d} ($d > 4$) are denoted irrelevant operators. The scale Λ can be the mass of a heavy field (e.g., M_W in the Fermi theory of weak interactions) or it reflects the short-distance structure in a more indirect way.

2. *Partial decoupling* In contrast to the previous case, the heavy fields do not disappear completely from the EFT but only their high-momentum modes are integrated out. The main area of application is the physics of heavy quarks. The procedure involves one or several field redefinitions introducing a frame dependence. Lorentz invariance is not manifest but implies relations between coupling constants of the EFT (reparametrization invariance).

3. *Spontaneous symmetry breaking* The transition from the fundamental to the effective level occurs via a phase transition due to spontaneous symmetry breaking generating (pseudo-)Goldstone bosons. A spontaneously broken symmetry relates processes with different numbers of Goldstone bosons. Therefore, the distinction between renormalizable ($d \leq 4$) and nonrenormalizable ($d > 4$) parts in the effective Lagrangian [1] becomes meaningless. The effective Lagrangian of type 3 is generically nonrenormalizable. Nevertheless, such Lagrangians define perfectly consistent quantum field theories at sufficiently low energies. Instead of the operator dimension as in [1], the number of derivatives of the fields and the number of symmetry-breaking

insertions distinguish successive terms in the Lagrangian. The general structure of effective Lagrangians with spontaneously broken symmetries is largely independent of the specific physical realization (universality). There are many examples in condensed matter physics, but the two main applications in particle physics are electroweak symmetry breaking and chiral perturbation theory (both discussed later) with the spontaneously broken global chiral symmetry of quantum chromodynamics QCD.

Another classification of EFTs is related to the status of their coupling constants.

- A. *Coupling constants can be determined by matching the EFT with the underlying theory at short distances.* The underlying theory is known and Green functions can be calculated perturbatively at energies $\sim \Lambda$ both in the fundamental and in the effective theory. Identifying a minimal set of Green functions fixes the coupling constants g_{i_d} in eqn [1] at the scale Λ . Renormalization group equations can then be used to run the couplings down to lower scales. The nonrenormalizable terms in the Lagrangian [1] can be fully included in the perturbative analysis.
- B. *Coupling constants are constrained by symmetries only.*
 - The underlying theory and therefore also the EFT coupling constants are unknown. This is the case of the standard model (SM) (see the next section). A perturbative analysis beyond leading order only makes sense for the known renormalizable part $\mathcal{L}_{d \leq 4}$. The nonrenormalizable terms suppressed by powers of Λ are considered at tree level only. The associated coupling constants g_{i_d} serve as bookmarks for new physics. Usually, but not always (cf., e.g., the subsection “Noncommutative spacetime”), the symmetries of $\mathcal{L}_{d \leq 4}$ are assumed to constrain the couplings.
 - The matching cannot be performed in perturbation theory even though the underlying theory is known. This is the generic situation for EFTs of type 3 involving spontaneous symmetry breaking. The prime example is chiral perturbation theory as the EFT of QCD at low energies.

The SM as an EFT

With the possible exception of the scalar sector to be discussed in the subsection “Electroweak symmetry breaking” the SM is very likely the renormalizable part of an EFT of type 1B. Except for nonzero neutrino masses, the SM Lagrangian $\mathcal{L}_{d \leq 4}$ in [1]

accounts for physics up to energies of roughly the Fermi scale $G_F^{-1/2} \simeq 300$ GeV.

Since the SM works exceedingly well up to the Fermi scale where the electroweak gauge symmetry is spontaneously broken it is natural to assume that the operators O_{i_d} with $d > 4$, made up from fields representing the known degrees of freedom and including a single Higgs doublet in the SM proper, should be gauge invariant with respect to the full SM gauge group $SU(3)_c \times SU(2)_L \times U(1)_Y$. An almost obvious constraint is Lorentz invariance that will be lifted in the next subsection, however.

These requirements limit the Lagrangian with operator dimension $d=5$ to a single term (except for generation multiplicity), consisting only of a left-handed lepton doublet L_L and the Higgs doublet Φ :

$$O_{d=5} = \epsilon_{ij} \epsilon_{kl} L_{iL}^\top C^{-1} L_{kL} \Phi_j \Phi_l + \text{h.c.} \quad [2]$$

This term violates lepton number and generates nonzero Majorana neutrino masses. For a neutrino mass of 1 eV, the scale Λ would have to be of the order of 10^{13} GeV if the associated coupling constant in the EFT Lagrangian [1] is of order 1.

In contrast to the simplicity for $d=5$, the list of gauge-invariant operators with $d=6$ is enormous. Among them are operators violating baryon or lepton number that must be associated with a scale much larger than 1 TeV. To explore the territory close to present energies, it therefore makes sense to impose baryon and lepton number conservation on the operators with $d=6$. Those operators have all been classified (Buchmüller and Wyler 1986) and the number of independent terms is of the order of 80. They can be grouped in three classes.

The first class consists of gauge and Higgs fields only. The corresponding EFT Lagrangian has been used to parametrize new physics in the gauge sector constrained by precision data from LEP. The second class consists of operators bilinear in fermion fields, with additional gauge and Higgs fields to generate $d=6$. Finally, there are four-fermion operators without other fields or derivatives. Some of the operators in the last two groups are also constrained by precision experiments, with a certain hierarchy of limits. For lepton and/or quark flavor conserving terms, the best limits on Λ are in the few TeV range, whereas the absence of neutral flavor changing processes yields lower bounds on Λ that are several orders of magnitude larger. If there is new physics in the TeV range flavor changing neutral transitions must be strongly suppressed, a powerful constraint on model building.

It is amazing that the most general renormalizable Lagrangian with the given particle content accounts

for almost all experimental results in such an impressive manner. Finally, we recall that many of the operators of dimension 6 are also generated in the SM via radiative corrections. A necessary condition for detecting evidence for new physics is therefore that the theoretical accuracy of radiative corrections matches or surpasses the experimental precision.

Noncommutative Spacetime

Noncommutative geometry arises in some string theories and may be expected on general grounds when incorporating gravity into a quantum field theory framework. The natural scale of noncommutative geometry would be the Planck scale in this case without observable consequences at presently accessible energies. However, as in theories with large extra dimensions the characteristic scale Λ_{NC} could be significantly smaller. In parallel to theoretical developments to define consistent noncommutative quantum field theories (short for quantum field theories on noncommutative spacetime), a number of phenomenological investigations have been performed to put lower bounds on Λ_{NC} .

Noncommutative geometry is a deformation of ordinary spacetime where the coordinates, represented by Hermitian operators \hat{x}_μ , do not commute:

$$[\hat{x}_\mu, \hat{x}_\nu] = i\theta_{\mu\nu} \quad [3]$$

The antisymmetric real tensor $\theta_{\mu\nu}$ has dimensions length^2 and it can be interpreted as parametrizing the resolution with which spacetime can be probed. In practically all applications, $\theta_{\mu\nu}$ has been assumed to be a constant tensor and we may associate an energy scale Λ_{NC} with its nonzero entries:

$$\Lambda_{\text{NC}}^{-2} \sim \theta_{\mu\nu} \quad [4]$$

There is to date no unique form for the noncommutative extension of the SM. Nevertheless, possible observable effects of noncommutative geometry have been investigated. Not unexpected from an EFT point of view, for energies $\ll \Lambda_{\text{NC}}$, noncommutative field theories are equivalent to ordinary quantum field theories in the presence of nonstandard terms containing $\theta_{\mu\nu}$ (Seiberg–Witten map). Practically all applications have concentrated on effects linear in $\theta_{\mu\nu}$.

Kinetic terms in the Lagrangian are in general unaffected by the noncommutative structure. New effects arise therefore mainly from renormalizable $d=4$ interactions terms. For example, the Yukawa coupling $g_Y \bar{\psi}\psi\phi$ generates the following interaction linear in $\theta_{\mu\nu}$:

$$\mathcal{L}_Y^{\text{NC}} = g_Y \theta_{\mu\nu} (\partial^\mu \bar{\psi} \partial^\nu \psi \phi + \partial^\mu \bar{\psi} \psi \partial^\nu \phi + \bar{\psi} \partial^\mu \psi \partial^\nu \phi) \quad [5]$$

These interaction terms have operator dimension 6 and they are suppressed by $\theta_{\mu\nu} \sim \Lambda_{\text{NC}}^{-2}$. The major difference to the previous discussion on physics beyond the SM is that there is an intrinsic violation of Lorentz invariance due to the constant tensor $\theta_{\mu\nu}$. In contrast to the previous analysis, the terms with dimension $d > 4$ do not respect the symmetries of the SM.

If $\theta_{\mu\nu}$ is indeed constant over macroscopic distances, many tests of Lorentz invariance can be used to put lower bounds on Λ_{NC} . Among the exotic effects investigated are modified dispersion relations for particles, decay of high-energy photons, charged particles producing Cerenkov radiation in vacuum, birefringence of radiation, a variable speed of light, etc. A generic signal of noncommutativity is the violation of angular momentum conservation that can be searched for at the Large Hadron Collider (LHC) and at the next linear collider.

Lacking a unique noncommutative extension of the SM, unambiguous lower bounds on Λ_{NC} are difficult to establish. However, the range $\Lambda_{\text{NC}} \lesssim 10 \text{ TeV}$ is almost certainly excluded. An estimate of the induced electric dipole moment of the electron (noncommutative field theories violate CP in general to first order in $\theta_{\mu\nu}$) yields $\Lambda_{\text{NC}} \gtrsim 100 \text{ TeV}$. On the other hand, if the SM were CP invariant, noncommutative geometry would be able to account for the observed CP violation in $K^0 - \bar{K}^0$ mixing for $\Lambda_{\text{NC}} \sim 2 \text{ TeV}$.

Electroweak Symmetry Breaking

In the SM, electroweak symmetry breaking is realized in the simplest possible way through renormalizable interactions of a scalar Higgs doublet with gauge bosons and fermions, a gauged version of the linear σ model.

The EFT version of electroweak symmetry breaking (EWEFT) uses only the experimentally established degrees of freedom in the SM (fermions and gauge bosons). Spontaneous gauge symmetry breaking is realized nonlinearly, without introducing additional scalar degrees of freedom. It is a low-energy expansion where energies and masses are assumed to be small compared to the symmetry-breaking scale. From both perturbative and nonperturbative arguments we know that this scale cannot be much bigger than 1 TeV. The Higgs model can be viewed as a specific example of an EWEFT as long as the Higgs boson is not too light (heavy-Higgs scenario).

The lowest-order effective Lagrangian takes the following form:

$$\mathcal{L}_{\text{EWSB}}^{(2)} = \mathcal{L}_B + \mathcal{L}_F \quad [6]$$

where \mathcal{L}_F contains the gauge-invariant kinetic terms for quarks and leptons including mass terms. In addition to the kinetic terms for the gauge bosons W_μ, B_μ , the bosonic Lagrangian \mathcal{L}_B contains the characteristic lowest-order term for the would-be-Goldstone bosons:

$$\mathcal{L}_B = \mathcal{L}_{\text{gauge}}^{\text{kin}} + \frac{v^2}{4} \langle D_\mu U^\dagger D^\mu U \rangle \quad [7]$$

with the gauge-covariant derivative

$$\begin{aligned} D_\mu U &= \partial_\mu U - ig W_\mu U + ig' U \hat{B}_\mu \\ W_\mu &= \frac{\vec{\tau}}{2} W_\mu, \quad \hat{B}_\mu = \frac{\tau_3}{2} B_\mu \end{aligned} \quad [8]$$

where $\langle \dots \rangle$ denotes a (two-dimensional) trace. The matrix field $U(\phi)$ carries the nonlinear representation of the spontaneously broken gauge group and takes the value $U=1$ in the unitary gauge. The Lagrangian [6] is invariant under local $SU(2)_L \times U(1)_Y$ transformations:

$$\begin{aligned} W_\mu &\rightarrow g_L W_\mu g_L^\dagger + \frac{i}{g} g_L \partial_\mu g_L^\dagger \\ \hat{B}_\mu &\rightarrow \hat{B}_\mu + \frac{i}{g'} g_R \partial_\mu g_R^\dagger \\ f_L &\rightarrow g_L f_L, \quad f_R \rightarrow g_R f_R, \quad U \rightarrow g_L U g_R^\dagger \end{aligned} \quad [9]$$

with

$$\begin{aligned} g_L(x) &= \exp(i\vec{\alpha}_L(x)\vec{\tau}/2) \\ g_R(x) &= \exp(i\alpha_Y(x)\tau_3/2) \end{aligned}$$

and $f_{L(R)}$ are quark and lepton fields grouped in doublets.

As is manifest in the unitary gauge $U=1$, the lowest-order Lagrangian of the EWEFT just implements the tree-level masses of gauge bosons ($M_W = M_Z \cos \theta_W = vg/2$, $\tan \theta_W = g'/g$) and fermions but does not carry any further information about the underlying mechanism of spontaneous gauge symmetry breaking. This information is first encoded in the couplings a_i of the next-to-leading-order Lagrangian

$$\mathcal{L}_{\text{EWSB}}^{(4)} = \sum_{i=0}^{14} a_i O_i \quad [10]$$

with monomials O_i of $O(p^4)$ in the low-energy expansion. The Lagrangian [10] is the most general CP and $SU(2)_L \times U(1)_Y$ invariant Lagrangian of $O(p^4)$.

Instead of listing the full Lagrangian, we display three typical examples:

$$\begin{aligned} O_0 &= \frac{v^2}{4} \langle TV_\mu \rangle^2 \\ O_3 &= -g \langle W_{\mu\nu} [V^\mu, V^\nu] \rangle \\ O_5 &= \langle V_\mu V^\mu \rangle^2 \end{aligned} \quad [11]$$

where

$$\begin{aligned} T &= U\tau_3 U^\dagger, \quad V_\mu = D_\mu U U^\dagger \\ W_{\mu\nu} &= \frac{i}{g} [\partial_\mu - ig W_\mu, \partial_\nu - ig W_\nu] \end{aligned} \quad [12]$$

In the unitary gauge, the monomials O_i reduce to polynomials in the gauge fields. The three examples in eqn [11] start with quadratic, cubic, and quartic terms in the gauge fields, respectively. The strongest constraints exist for the coefficients of quadratic contributions from the Large Electron-Positron collider LEP1, less restrictive ones for the cubic self-couplings from LEP2, and none so far for the quartic ones.

Heavy-Quark Physics

EFTs in this section are derived from the SM and they are of type 2A in the classification introduced previously. In a first step, one integrates out W, Z , and top quark. Evolving down from M_W to m_b , large logarithms $\alpha_s(m_b) \ln(M_W^2/m_b^2)$ are resummed into the Wilson coefficients. At the scale of the b -quark, QCD is still perturbative, so that at least a part of the amplitudes is calculable in perturbation theory. To separate the calculable part from the rest, the EFTs below perform an expansion in $1/m_Q$, where m_Q is the mass of the heavy quark.

Heavy-quark EFTs offer several important advantages.

1. Approximate symmetries that are hidden in full QCD appear in the expansion in $1/m_Q$.
2. Explicit calculations simplify in general, for example, the summing of large logarithms via renormalization group equations.
3. The systematic separation of hard and soft effects for certain matrix elements (factorization) can be achieved much more easily.

Heavy-Quark Effective Theory

Heavy-quark effective theory (HQET) is reminiscent of the Foldy-Wouthuysen transformation (nonrelativistic expansion of the Dirac equation). It is a systematic expansion in $1/m_Q$, when $m_Q \gg \Lambda_{\text{QCD}}$, the scale parameter of QCD. It can be applied to processes where the heavy quark remains essentially on shell: its velocity v changes only by small amounts $\sim \Lambda_{\text{QCD}}/m_Q$. In the hadron rest frame, the heavy quark is almost at rest and acts as a quasistatic source of gluons.

More quantitatively, one writes the heavy-quark momentum as $p^\mu = m_Q v^\mu + k^\mu$, where v is the hadron 4-velocity ($v^2=1$) and k is a residual

momentum of $O(\Lambda_{\text{QCD}})$. The heavy quark field $Q(x)$ is then decomposed with the help of energy projectors $P_v^\pm = (1 \pm \not{v})/2$ and employing a field redefinition:

$$\begin{aligned} Q(x) &= e^{-im_Q v \cdot x} (h_v(x) + H_v(x)) \\ h_v(x) &= e^{im_Q v \cdot x} P_v^+ Q(x) \\ H_v(x) &= e^{im_Q v \cdot x} P_v^- Q(x) \end{aligned} \quad [13]$$

In the hadron rest frame, $h_v(x)$ and $H_v(x)$ correspond to the upper and lower components of $Q(x)$, respectively. With this redefinition, the heavy-quark Lagrangian is expressed in terms of a massless field h_v and a “heavy” field H_v :

$$\begin{aligned} \mathcal{L}_Q &= \bar{Q}(i\not{D} - m_Q)Q \\ &= \bar{h}_v i\not{v} \cdot D h_v - \bar{H}_v (i\not{v} \cdot D + 2m_Q) H_v \\ &\quad + \text{mixed terms} \end{aligned} \quad [14]$$

At the semiclassical level, the field H_v can be eliminated by using the QCD field equation $(i\not{D} - m_Q)Q = 0$ yielding the nonlocal expression

$$\mathcal{L}_Q = \bar{h}_v i\not{v} \cdot D h_v + \bar{h}_v i\not{D}_\perp \frac{1}{i\not{v} \cdot D + 2m_Q - i\epsilon} i\not{D}_\perp h_v \quad [15]$$

with $D_\perp^\mu = (g^{\mu\nu} - v^\mu v^\nu) D_\nu$. The field redefinition in [13] ensures that, in the heavy-hadron rest frame, derivatives of h_v give rise to small momenta of $O(\Lambda_{\text{QCD}})$ only. The Lagrangian [15] is the starting point for a systematic expansion in m_Q .

To leading order in $1/m_Q$ ($Q = b, c$), the Lagrangian

$$\mathcal{L}_{b,c} = \bar{b}_v i\not{v} \cdot D b_v + \bar{c}_v i\not{v} \cdot D c_v \quad [16]$$

exhibits two important approximate symmetries of HQET: the flavor symmetry $\text{SU}(2)_F$ relating heavy quarks moving with the same velocity and the heavy-quark spin symmetry generating an overall $\text{SU}(4)$ spin-flavor symmetry. The flavor symmetry is obvious and the spin symmetry is due to the absence of Dirac matrices in [16]: both spin degrees of freedom couple to gluons in the same way. The simplest spin-symmetry doublet consists of a pseudoscalar meson H and the associated vector meson H^* . Denoting the doublet by \mathcal{H} , the matrix elements of the heavy-to-heavy transition current are determined to leading order in $1/m_Q$ by a single form factor, up to Clebsch–Gordan coefficients:

$$\langle \mathcal{H}(v') | \bar{h}_v \Gamma h_v | \mathcal{H}(v) \rangle \sim \xi(v \cdot v') \quad [17]$$

Γ is an arbitrary combination of Dirac matrices and the form factor ξ is the so-called Isgur–Wise function. Moreover, since $\bar{h}_v \gamma^\mu h_v$ is the Noether current of heavy-flavor symmetry, the Isgur–Wise function is fixed in the no-recoil limit $v' = v$ to be

$\xi(v \cdot v' = 1) = 1$. The semileptonic decays $B \rightarrow D l \nu_l$ and $B \rightarrow D^* l \nu_l$ are therefore governed by a single normalized form factor to leading order in $1/m_Q$, with important consequences for the determination of the Cabibbo–Kobayashi–Maskawa (CKM) matrix element V_{cb} .

The HQET Lagrangian is superficially frame dependent. Since the SM is Lorentz invariant, the HQET Lagrangian must be independent of the choice of the frame vector v . Therefore, a shift in v accompanied by corresponding shifts of the fields h_v and of the covariant derivatives must leave the Lagrangian invariant. This reparametrization invariance is unaffected by renormalization and it relates coefficients with different powers in $1/m_Q$.

Soft-Collinear Effective Theory

HQET is not applicable in heavy-quark decays where some of the light particles in the final state have momenta of $O(m_Q)$, for example, for inclusive decays like $B \rightarrow X_s \gamma$ or exclusive ones like $B \rightarrow \pi\pi$. In recent years, a systematic heavy-quark expansion for heavy-to-light decays has been set up in the form of soft-collinear effective theory (SCET).

SCET is more complicated than HQET because now the low-energy theory involves more than one scale. In the SCET Lagrangian, a light quark or gluon field is represented by several effective fields. In addition to the soft fields h_v in [15], the so-called collinear fields enter that have large energy and carry large momentum in the direction of the light hadrons in the final state.

In addition to the frame vector v of HQET ($v = (1, 0, 0, 0)$ in the heavy-hadron rest frame), SCET introduces a lightlike reference vector n in the direction of the jet of energetic light particles (for inclusive decays), for example, $n = (1, 0, 0, 1)$. All momenta p are decomposed in terms of light-cone coordinates (p_+, p_-, p_\perp) with

$$p^\mu = \frac{n \cdot p}{2} \bar{n}^\mu + \frac{\bar{n} \cdot p}{2} n^\mu + p_\perp^\mu = p_+^\mu + p_-^\mu + p_\perp^\mu \quad [18]$$

where $\bar{n} = 2v - n = (1, 0, 0, -1)$. For large energies, the three light-cone components are widely separated, with $p_- = O(m_Q)$ being large while p_\perp and p_+ are small. Introducing a small parameter $\lambda \sim p_\perp/p_-$, the light-cone components of (hard-)collinear particles scale like $(p_+, p_-, p_\perp) = m_Q(\lambda^2, 1, \lambda)$. Thus, there are three different scales in the problem compared to only two in HQET. For exclusive decays, the situation is even more involved.

The SCET Lagrangian is obtained from the full theory by an expansion in powers of λ . In addition to the heavy quark field h_v , one introduces soft as well as collinear quark and gluon fields by field

redefinitions so that the various fields have momentum components that scale appropriately with λ .

Similar to HQET, the leading-order Lagrangian of SCET exhibits again approximate symmetries that can lead to a reduction of form factors describing heavy-to-light decays. As in HQET, reparametrization invariance implements Lorentz invariance and results in stringent constraints on subleading corrections in SCET.

An important result of SCET is the proof of factorization theorems to all orders in α_s . For inclusive decays, the differential rate is of the form

$$d\Gamma \sim HJ \times S \quad [19]$$

where H contains the hard corrections. The so-called jet function J sensitive to the collinear region is convoluted with the shape function S representing the soft contributions. At leading order, the shape function drops out in the ratio of weighted decay spectra for $B \rightarrow X_u l \nu_l$ and $B \rightarrow X_s \gamma$ allowing for a determination of the CKM matrix element V_{ub} . Factorization theorems have become available for an increasing number of processes, most recently also for exclusive decays of B into two light mesons.

Nonrelativistic QCD

In HQET the kinetic energy of the heavy quark appears as a small correction of $O(\Lambda_{\text{QCD}}^2/m_Q)$. For systems with more than one heavy quark, the kinetic energy cannot be treated as a perturbation in general. For instance, the virial theorem implies that the kinetic energy in quarkonia $\bar{Q}Q$ is of the same order as the binding energy of the bound state.

NRQCD, the EFT for heavy quarkonia, is an extension of HQET. The Lagrangian for NRQCD coincides with HQET in the bilinear sector of the heavy-quark fields but it also includes quartic interactions between quarks and antiquarks. The relevant expansion parameter in this case is the relative velocity between Q and \bar{Q} . In contrast to HQET, there are at least three widely separate scales in heavy quarkonia: in addition to m_Q , the relative momentum of the bound quarks $p \sim m_Q v$ with $v \ll 1$ and the typical kinetic energy $E \sim m_Q v^2$. The main challenges are to derive the quark–antiquark potential directly from QCD and to describe quarkonium production and decay at collider experiments. In the abelian case, the corresponding EFT for quantum electrodynamics (QED) is called NRQED that has been used to study electromagnetically bound systems like the hydrogen atom, positronium, muonium, etc.

In NRQCD only the hard degrees of freedom with momenta $\sim m_Q$ are integrated out. Therefore, NRQCD is not enough for a systematic computation

of heavy-quarkonium properties. Because the non-relativistic fluctuations of order $m_Q v$ and $m_Q v^2$ have not been separated, the power counting in NRQCD is ambiguous in higher orders.

To overcome those deficiencies, two approaches have been put forward: potential NRQCD (pNRQCD) and velocity NRQCD (vNRQCD). In pNRQCD, a two-step procedure is employed for integrating out quark and gluon degrees of freedom:

$$\begin{array}{ccc} \text{QCD} & & \Lambda > m_Q \\ & \Downarrow & \\ \text{NRQCD} & & m_Q > \Lambda > m_Q v \\ & \Downarrow & \\ \text{pNRQCD} & & m_Q v > \Lambda > m_Q v^2 \end{array}$$

The resulting EFT derives its name from the fact that the four-quark interactions generated in the matching procedure are the potentials that can be used in Schrödinger perturbation theory. It is claimed that pNRQCD can also be used in the nonperturbative domain where $\alpha_s(m_Q v^2)$ is of order 1 or larger. The advantage would be that also charmonium becomes accessible to a systematic EFT analysis.

The alternative approach of vNRQCD is only applicable in the fully perturbative regime when $m_Q \gg m_Q v \gg m_Q v^2 \gg \Lambda_{\text{QCD}}$ is valid. It separates the different degrees of freedom in a single step leaving only ultrasoft energies and momenta of $O(m_Q v^2)$ as continuous variables. The separation of larger scales proceeds in a similar fashion as in HQET via field redefinitions. A systematic nonrelativistic power counting in the velocity v is implemented.

The Standard Model at Low Energies

At energies below 1 GeV, hadrons – rather than quarks and gluons – are the relevant degrees of freedom. Although the strong interactions are highly nonperturbative in the confinement region, Green functions and amplitudes are amenable to a systematic low-energy expansion. The key observation is that the QCD Lagrangian with $N_f = 2$ or 3 light quarks,

$$\begin{aligned} \mathcal{L}_{\text{QCD}} &= \bar{q}(i\not{D} - \mathcal{M}_q)q - \frac{1}{4}G_{\mu\nu}^\alpha G^{\alpha\mu\nu} + \mathcal{L}_{\text{heavy quarks}} \\ &= \bar{q}_L i\not{D} q_L + \bar{q}_R i\not{D} q_R - \bar{q}_L \mathcal{M}_q q_R \\ &\quad - \bar{q}_R \mathcal{M}_q q_L + \dots \\ q_{R,L} &= \frac{1}{2}(1 \pm \gamma_5)q, \quad q^\top = (ud[s]) \end{aligned} \quad [20]$$

exhibits a global symmetry

$$\underbrace{\text{SU}(N_f)_L \times \text{SU}(N_f)_R}_{\text{chiral group } G} \times \text{U}(1)_V \times \text{U}(1)_A \quad [21]$$

in the limit of N_f massless quarks ($\mathcal{M}_q = 0$). At the hadronic level, the quark number symmetry $U(1)_V$ is realized as baryon number. The axial $U(1)_A$ is not a symmetry at the quantum level due to the abelian anomaly.

Although not yet derived from first principles, there are compelling theoretical and phenomenological arguments that the ground state of QCD is not even approximately chirally symmetric. All evidence, such as the existence of relatively light pseudoscalar mesons, points to spontaneous chiral symmetry breaking $G \rightarrow SU(N_f)_V$, where $SU(N_f)_V$ is the diagonal subgroup of G . The resulting $N_f^2 - 1$ (pseudo-)Goldstone bosons interact weakly at low energies. In fact, Goldstone's theorem ensures that purely mesonic or single-baryon amplitudes vanish in the chiral limit ($\mathcal{M}_q = 0$) when the momenta of all pseudoscalar mesons tend to zero. This is the basis for a systematic low-energy expansion of Green functions and amplitudes. The corresponding EFT (type 3B in our classification) is called chiral perturbation theory (CHPT) (Weinberg 1979, Gasser and Leutwyler 1984, 1985).

Although the construction of effective Lagrangians with nonlinearly realized chiral symmetry is well understood, there are some subtleties involved. First of all, there may be terms in a chiral-invariant action that cannot be written as the four-dimensional integral of an invariant Lagrangian. The chiral anomaly for $SU(3) \times SU(3)$ bears witness of this fact and gives rise to the Wess–Zumino–Witten action. A general theorem to account for such exceptional cases is due to D'Hoker and Weinberg (1994). Consider the most general action for Goldstone fields with symmetry group G , spontaneously broken to a subgroup H . The only possible non- G -invariant terms in the Lagrangian that give rise to a G -invariant action are in one-to-one correspondence with the generators of the fifth cohomology group $\mathcal{H}^5(G/H; \mathbb{R})$ of the coset manifold G/H . For the relevant case of chiral $SU(N)$, the coset space $SU(N)_L \times SU(N)_R / SU(N)_V$ is itself an $SU(N)$ manifold. For $N \geq 3$, $\mathcal{H}^5(SU(N); \mathbb{R})$ has a single generator that corresponds precisely to the Wess–Zumino–Witten term.

At a still deeper level, one may ask whether chiral-invariant Lagrangians are sufficient (except for the anomaly) to describe the low-energy structure of Green functions as dictated by the chiral Ward identities of QCD. To be able to calculate such Green functions in general, the global chiral symmetry of QCD is extended to a local symmetry by the introduction of external gauge fields. The following invariance theorem (Leutwyler 1994) provides an answer to the above question. Except

for the anomaly, the most general solution of the Ward identities for a spontaneously broken symmetry in Lorentz-invariant theories can be obtained from gauge-invariant Lagrangians to all orders in the low-energy expansion. The restriction to Lorentz invariance is crucial: the theorem does not hold in general in nonrelativistic effective theories.

Chiral Perturbation Theory

The effective chiral Lagrangian of the SM in the meson sector is displayed in Table 1. The lowest-order Lagrangian for the purely strong interactions is given by

$$\mathcal{L}_{p^2} = \frac{F^2}{4} \langle D_\mu U D^\mu U^\dagger \rangle + \frac{F^2 B}{2} \langle (s + ip) U^\dagger + (s - ip) U \rangle \quad [22]$$

with a covariant derivative $D = \partial_\mu U - i(v_\mu + a_\mu)U + iU(v_\mu - a_\mu)$. The first term has the familiar form [7] of the gauged nonlinear σ model, with the matrix field $U(\phi)$ transforming as $U \rightarrow g_R U g_L^\dagger$ under chiral rotations. External fields v_μ, a_μ, s, p are introduced for constructing the generating functional of Green functions of quark currents. To implement explicit chiral symmetry breaking, the scalar field s is set equal to the quark mass matrix \mathcal{M}_q at the end of the calculation.

The leading-order Lagrangian has two free parameters F, B related to the pion decay constant and to the quark condensate, respectively:

$$F_\pi = F[1 + O(m_q)] \quad [23]$$

$$\langle 0 | \bar{u}u | 0 \rangle = -F^2 B[1 + O(m_q)]$$

The Lagrangian [22] gives rise to $M_\pi^2 = B(m_u + m_d)$ at lowest order. From detailed studies of pion-pion scattering (Colangelo *et al.* 2001), we know that the leading term accounts for at least 94% of the pion mass. This supports the standard counting of CHPT,

Table 1 The effective chiral Lagrangian of the SM in the meson sector

$\mathcal{L}_{\text{chiral order}} (\# \text{ of LECs})$	Loop order
$\mathcal{L}_{p^2}(2) + \mathcal{L}_{G_F p^2}^{\Delta S=1}(2) + \mathcal{L}_{e^2 p^0}^{\text{em}}(1) + \mathcal{L}_{G_8 e^2 p^0}^{\text{emweak}}(1)$	$L=0$
$+ \mathcal{L}_{p^4}(10) + \mathcal{L}_{p^6}^{\text{odd}}(32) + \mathcal{L}_{G_8 p^4}^{\Delta S=1}(22) + \mathcal{L}_{G_{27} p^4}^{\Delta S=1}(28)$	$L=1$
$+ \mathcal{L}_{e^2 p^2}^{\text{em}}(14) + \mathcal{L}_{G_8 e^2 p^2}^{\text{emweak}}(14) + \mathcal{L}_{e^2 p}^{\text{leptons}}(5)$	
$+ \mathcal{L}_{p^6}(90)$	$L=2$

The numbers in brackets refer to the number of independent couplings for $N_f = 3$. The parameter-free Wess–Zumino–Witten action S_{WZW} that cannot be written as the four-dimensional integral of an invariant Lagrangian must be added.

with quark masses booked as $O(p^2)$ like the two-derivative term in [22].

The effective chiral Lagrangian in Table 1 contains the following parts:

1. strong interactions: $\mathcal{L}_{p^2}, \mathcal{L}_{p^4}, \mathcal{L}_{p^6}^{\text{odd}}, \mathcal{L}_{p^6} + S_{\text{WZW}}$;
2. nonleptonic weak interactions to first order in the Fermi coupling constant G_F : $\mathcal{L}_{G_F p^2}^{\Delta S=1}, \mathcal{L}_{G_8 p^4}^{\Delta S=1}, \mathcal{L}_{G_{27} p^4}^{\Delta S=1}$;
3. radiative corrections for strong processes: $\mathcal{L}_{e^2 p^0}^{\text{em}}, \mathcal{L}_{e^2 p^2}^{\text{em}}$;
4. radiative corrections for nonleptonic weak decays: $\mathcal{L}_{G_8 e^2 p^0}^{\text{emweak}}, \mathcal{L}_{G_8 e^2 p^2}^{\text{emweak}}$; and
5. radiative corrections for semileptonic weak decays: $\mathcal{L}_{e^2 p}^{\text{leptons}}$.

Beyond the leading order, unitarity and analyticity require the inclusion of loop contributions. In the purely strong sector, calculations have been performed up to next-to-next-to-leading order. Figure 1 shows the corresponding skeleton diagrams of $O(p^6)$, with full lowest-order tree structures to be attached to propagators and vertices. The coupling constants of the various Lagrangians in Table 1 absorb the divergences from loop diagrams leading to finite renormalized Green functions with scale-dependent couplings, the so-called low-energy constants (LECs). As in all EFTs, the LECs parametrize the effect of “heavy” degrees of freedom that are not represented explicitly in the EFT Lagrangian. Determination of those LECs is a major task for CHPT. In addition to phenomenological information, further theoretical input is needed. Lattice gauge theory has already furnished values for some LECs. To bridge the gap between the low-energy domain of CHPT and the perturbative domain of QCD, large- N_c motivated interpolations with meson resonance exchange have been used successfully to pin down some of the LECs.

Especially in cases where the knowledge of LECs is limited, renormalization group methods provide valuable information. As in renormalizable quantum field theories, the leading chiral logs $(\ln M^2/\mu^2)^L$

with a typical meson mass M , renormalization scale μ and loop order L can in principle be determined from one-loop diagrams only. In contrast to the renormalizable situation, new derivative structures (and quark mass insertions) occur at each loop order preventing a straightforward resummation of chiral logs.

Among the many applications of CHPT in the meson sector are the determination of quark mass ratios and the analysis of pion-pion scattering where the chiral amplitude of next-to-next-to-leading order has been combined with dispersion theory (Roy equations). Of increasing importance for precision physics (CKM matrix elements, $(g-2)_\mu, \dots$) are isospin-violating corrections including radiative corrections, where CHPT provides the only reliable approach in the low-energy region. Such corrections are also essential for the analysis of hadronic atoms like ponium, a $\pi^+\pi^-$ bound state.

CHPT has also been applied extensively in the single-baryon sector. There are several differences to the purely mesonic case. For instance, the chiral expansion proceeds more slowly and the nucleon mass m_N provides a new scale that does not vanish in the chiral limit. The formulation of heavy-baryon CHPT was modeled after HQET integrating out the nucleon modes of $O(m_N)$. To improve the convergence of the chiral expansion in some regions of phase space, a manifestly Lorentz-invariant formulation has been set up more recently (relativistic baryon CHPT). Many single-baryon processes have been calculated to fourth order in both approaches, for example, pion-nucleon scattering. With similar methods as in the mesonic sector, hadronic atoms like pionic or kaonic hydrogen have been investigated.

Nuclear Physics

In contrast to the meson and single-baryon sectors, amplitudes with two or more nucleons do not vanish in the chiral limit when the momenta of Goldstone mesons tend to zero. Consequently, the power counting is different in the many-nucleon sector. Multinucleon processes are treated with different EFTs depending on whether all momenta are smaller or larger than the pion mass.

In the very low energy regime $|\vec{p}| \ll M_\pi$, pions or other mesons do not appear as dynamical degrees of freedom. The resulting EFT is called “pionless EFT” and it describes systems like the deuteron, where the typical nucleon momenta are $\sim \sqrt{m_N B_d} \simeq 45 \text{ MeV}$ (B_d is the binding energy of the deuteron). The Lagrangian for the strong interactions between two nucleons has the form

$$\mathcal{L}_{NN} = C_0 (N^\top P_i N)^\dagger N^\top P_i N + \dots \quad [24]$$

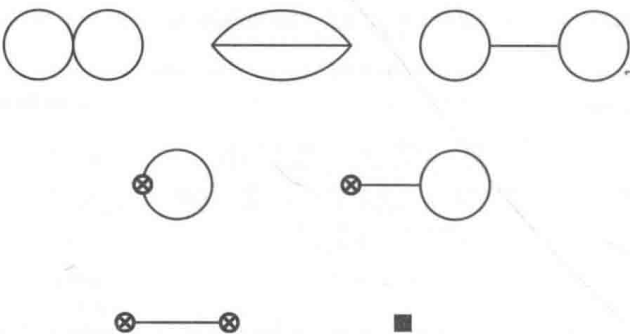


Figure 1 Skeleton diagrams of $O(p^6)$. Normal vertices are from \mathcal{L}_{p^2} , crossed circles and the full square denote vertices from \mathcal{L}_{p^4} and \mathcal{L}_{p^6} , respectively.

where P_i are spin–isospin projectors and higher-order terms contain derivatives of the nucleon fields. The existence of bound states implies that at least part of the EFT Lagrangian must be treated nonperturbatively. Pionless EFT is an extension of effective-range theory that has long been used in nuclear physics. It has been applied successfully especially to the deuteron but also to more complicated few-nucleon systems like the Nd and $n\alpha$ systems. For instance, precise results for Nd scattering have been obtained with parameters fully determined from NN scattering. Pionless EFT has also been applied to the so-called halo nuclei, where a tight cluster of nucleons (like ${}^4\text{He}$) is surrounded by one or more “halo” nucleons.

In the regime $|\vec{p}| > M_\pi$, the pion must be included as a dynamical degree of freedom. With some modifications in the power counting, the corresponding EFT is based on the approach of Weinberg (1990, 1991), who applied the usual rules of the meson and single-nucleon sectors to the nucleon–nucleon potential (instead of the scattering amplitude). The potential is then to be inserted into a Schrödinger equation to calculate physical observables. The systematic power counting leads to a natural hierarchy of nuclear forces, with only two-nucleon forces appearing up to next-to-leading order. Three- and four-nucleon forces arise at third and fourth order, respectively.

Significant progress has been achieved in the phenomenology of few-nucleon systems. The two- and n -nucleon ($3 \leq n \leq 6$) sectors have been pushed to fourth and third order, respectively, with encouraging signs of “convergence.” Compton scattering off the deuteron, πd scattering, nuclear parity violation, solar fusion, and other processes have been investigated in the EFT approach. The quark mass dependence of the nucleon–nucleon interaction has also been studied.

See also: Anomalies; Electroweak Theory; High T_c Superconductor Theory; Noncommutative Geometry and the Standard Model; Operator Product Expansion in Quantum Field Theory; Perturbation Theory and its Techniques; Quantum Chromodynamics; Quantum Electrodynamics and its Precision Tests; Renormalization: General Theory; Seiberg–Witten Theory; Standard Model of Particle Physics; Symmetries and Conservation Laws; Symmetry Breaking in Field Theory.

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Eigenfunctions of Quantum Completely Integrable Systems

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Introduction

This article is an introduction to eigenfunctions of quantum completely integrable (QCI) systems. For these systems, one can understand asymptotics of eigenfunctions better than for other systems, so it is natural to study them. It is useful to begin the discussion with the most important geometric example given by the quantum Hamiltonian, $P_1 = -\sqrt{\Delta}$. We fix a basis of eigenfunctions, $\varphi_j, j = 1, 2, \dots$, with

$$-\sqrt{\Delta}\varphi_j = \lambda_j\varphi_j, \quad \langle \varphi_i, \varphi_j \rangle = \delta_{ij}$$

and assume that there exist functionally independent (pseudo)differential operators P_2, \dots, P_n with the property that

$$[P_i, P_j] = 0, \quad i, j = 1, \dots, n$$

In this case, P_1 is said to be QCI and the operators, $P_k, k = 1, \dots, n$, can be simultaneously diagonalized. It is therefore natural to study the special basis of Laplace eigenfunctions which are joint eigenvectors of the P_k 's. From now on, the ϕ_j 's are always assumed to be joint eigenfunctions of the commuting operators, $P_k, k = 1, \dots, n$. The classical observables corresponding to the operators $P_k, k = 1, \dots, n$, are the respective principal symbols, $p_k \in C^\infty(T^*M), j = 1, \dots, n$. In particular, the bicharacteristic flow of $p_1(x, \xi) = |\xi|_g$ is the classical "geodesic flow"

$$G_t: T^*M \longrightarrow T^*M$$

Examples of manifolds with QCI Laplacians include tori and spheres of revolution, Liouville metrics on tori and spheres, large families of metrics on homogeneous spaces, as well as hyperellipsoids with distinct axes in arbitrary dimension. There are also many inhomogeneous QCI examples (see the next section). It is of interest to understand the asymptotics of both eigenvalues and eigenfunctions. There is a large literature devoted to eigenvalue asymptotics, including trace formulas and Bohr–Sommerfeld rules (see Colin de Verdiere (1994a, b), Helffer and Sjostrand (1990), and Colin de Verdiere and Vu Ngoc (2003)). We will concentrate here on the corresponding problem of determining eigenfunction asymptotics. The key property of eigenfunctions in the QCI case is localization in phase space, T^*M . This allows one to study more effectively the concentration and blow-up properties than in any other setting. It is important to contrast

this with, for example, the situation in the ergodic case. Moreover, in the QCI case, there is a particularly strong connection between dynamics of the geodesic flow, $G_t: T^*M \rightarrow T^*M$, and the asymptotics of individual eigenfunctions. In the general case, one can usually only relate the dynamics to spectral averages, such as in the trace formula (Duistermaat and Guillemin 1975).

For the most part, the literature on eigenfunction asymptotics addresses the following basic problems:

1. determining sharp upper and lower bounds for φ_j as $\lambda_j \rightarrow \infty$ and
2. describing the link between the blow-up properties of φ_j as $\lambda_j \rightarrow \infty$ and the dynamics of the geodesic flow, G_t .

The starting point in the study of eigenfunction asymptotics in the QCI case is the fact that the joint eigenfunctions, φ_j , have masses that localize on the level sets, $\mathcal{P}^{-1}(b) := \{(x, \xi) \in T^*M; p_j(x, \xi) = b_j, j = 1, \dots, n\}$. Moreover, by the Liouville–Arnol'd theorem, for generic levels (indexed by $b \in \mathbb{R}$),

$$\mathcal{P}^{-1}(b) = \sum_{k=1}^m \Lambda_k(b) \quad [1]$$

where the $\Lambda_k(b) \subset T^*M$ are Lagrangian tori. The affine symplectic coordinates in a neighborhood of $\Lambda_k(b)$ are called "action-angle variables" $(\theta_1^{(k)}, \dots, \theta_n^{(k)}; I_1^{(k)}, \dots, I_n^{(k)}) \in \mathbb{T}^n \times \mathbb{R}^n$. Written in terms of these coordinates, the classical Hamilton equations defining the geodesic flow assume the form

$$\frac{d\theta}{dt} = F(I), \quad \frac{dI}{dt} = 0$$

and this system of ordinary differential equations (ODEs) is solved by quadrature. This explains why one refers to such systems as completely integrable. At the quantum level, one can construct semiclassical Lagrangian distributions,

$$\Phi_\lambda(x) := \int_{\mathbb{R}^n} e^{i\lambda\varphi^{(k)}(x, \eta)} a(x, \eta; \lambda) d\eta \quad [2]$$

which microlocally concentrate on $\Lambda^{(k)}(b)$ as $\lambda \rightarrow \infty$ and satisfy $P_j\Phi_\lambda = b_j\lambda\Phi_\lambda + \mathcal{O}(\lambda^{-\infty})$ in $L^2(M)$. An important fact is that the actual joint eigenfunctions, φ_j , are approximated to $\mathcal{O}(\lambda^{-\infty})$ -accuracy in $L^2(M)$ by suitable linear combinations of the quasimodes, Φ_λ . However, there are subtleties underlying this correspondence which are often neglected in the physics literature:

3. The actual joint eigenfunctions ϕ_j localize on the level sets $\mathcal{P}^{-1}(b)$ which usually consist of many

connected components. Consequently, the eigenfunctions are approximated by (sometimes large) linear combinations of Lagrangian quasimodes attached to the different component tori. The precise splitting of mass amongst these different components is a difficult and, in general, unsolved problem in microlocal tunneling.

4. The local torus foliation given by action-angle variables tends to degenerate and Lagrangian quasimodes are no longer approximate solutions to the (joint) eigenvalue equations near the singularities of the foliation. The singularities and their relative configurations can be complicated (Colin de Verdiere and Vu Ngoc 2003) and most of the interesting asymptotic blow-up properties of eigenfunctions tend to be associated with these degeneracies. The main tool for studying joint eigenfunctions near degeneracies is the quantum analog of the Eliasson normal form (Eliasson 1984, Vu Ngoc 2000). We will refer to this as the “quantum Birkhoff normal form” (QBNF).

Background on QCI Systems

Let (M^n, g) be a compact, closed Riemannian manifold and $P_1 := Op_b(p_1)$ be a formally self-adjoint, elliptic (in the classical sense) \hbar -pseudodifferential operator. In local coordinates, the Schwarz kernel of P_1 is of the form,

$$P_1(x, y; \hbar) = (2\pi\hbar)^{-n} \int_{\mathbb{R}^n} e^{i\langle x-y, \xi \rangle / \hbar} p_1(x, \xi; \hbar) d\xi$$

where $p_1(x, \xi; \hbar) \in S_{cl}^{0, m}(T^*M)$; that is, $p_1(x, \xi; \hbar) \sim \sum_{j=0}^{\infty} p_{1,j}(x, \xi) \hbar^j$ with $\partial_x^\alpha \partial_\xi^\beta p_{1,j}(x, \xi) = \mathcal{O}_{\alpha, \beta}(\langle \xi \rangle^{m-j-|\beta|})$ (Dimassi and Sjostrand 1999). It is often convenient to work with \hbar -pseudodifferential operators rather than their classical counterparts. In the homogeneous case, one chooses $\hbar^{-1} \in \text{Spec} \sqrt{\Delta}$.

$P_1 \in Op_b(S_{cl}^{0, m})$ is said to be QCI if there exist self-adjoint $P_j = Op_b(p_j) \in Op_b(S_{cl}^{0, m'})$, $j = 2, \dots, n$, for some m' with $[P_i, P_j] = 0$, $i, j = 1, \dots, n$, such that $dp_1 \wedge \dots \wedge dp_n \neq 0$ on a dense open subset, $\Omega_{reg} \subset T^*M$, and $P_1^2 + \dots + P_n^2$ is elliptic in the classical sense. There are many inhomogeneous QCI examples including quantum Euler, Lagrange, and Kowalevsky tops together with quantum Neumann and Rosocha-tius oscillators in arbitrary dimension.

Since $\{p_i, p_j\} = 0$, the joint Hamilton flow of the p_i 's induces a symplectic \mathbb{R}^n -action on T^*M :

$$\begin{aligned} \Phi_t : T^*M &\longrightarrow T^*M \\ \Phi_t(x, \xi) &= \exp t_1 H_{p_1} \circ \dots \circ \exp t_n H_{p_n}(x, \xi) \\ t &= (t_1, \dots, t_n) \in \mathbb{R}^n \end{aligned}$$

The associated moment map is just

$$\mathcal{P} : T^*M - 0 \rightarrow \mathbb{R}^n, \quad \mathcal{P} = (p_1, \dots, p_n)$$

We denote the image $\mathcal{P}(T^*M - 0)$ by \mathcal{B} , the regular values (resp. singular values) by \mathcal{B}_{reg} (resp. \mathcal{B}_{sing}) of the moment map.

To establish bounds for the joint eigenfunctions of P_1, \dots, P_n , one imposes a “finite-complexity” assumption (Toth and Zelditch 2002) on the classical integrable system. This condition holds for all systems of interest in physics. To describe it, for each $b = (b^{(1)}, \dots, b^{(n)}) \in \mathcal{B}$, let $m_{cl}(b)$ denote the number of \mathbb{R}^n -orbits of the joint flow Φ_t on the level set $\mathcal{P}^{-1}(b)$. Then, the finite-complexity condition says that for some $M_0 > 0$,

$$m_{cl}(b) < M_0 (\forall b \in \mathcal{B})$$

In addition, when \mathcal{P} is proper,

$$\mathcal{P}^{-1}(b) = \sum_{k=1}^{m_{cl}(b)} \Lambda_k(b) \quad [3]$$

for any $b \in \mathcal{B}_{reg}$, where the $\Lambda_k(b)$ are Lagrangian tori. The starting point for analyzing joint eigenfunctions is the following correspondence principle (Zelditch 1990) which makes the eigenfunction localization alluded to in the introduction more precise:

Theorem 1 *Let $Op_b(a) \in Op_b(S_{cl}^0)(T^*M)$ and $P_j, j = 1, \dots, n$, be a QCI system of commuting operators. Then, for every $b \in \mathcal{B}_{reg}$, there exists a subsequence of joint eigenfunctions $\varphi_\mu(x) := \varphi(x; \mu(\hbar))$ with $\hbar \in (0, \hbar_0]$ and joint eigenvalues $\mu(\hbar) = (\mu_1(\hbar), \dots, \mu_n(\hbar)) \in \text{Spec}(P_1, \dots, P_n)$ with $|\mu(\hbar) - b| = \mathcal{O}(\hbar)$ such that*

$$\langle Op_b(a) \varphi_\mu, \varphi_\mu \rangle = |c(\hbar)|^2 \int_{\Lambda(b)} a(x, \xi) d\mu_b + \mathcal{O}(\hbar)$$

Here, $d\mu_b$ denotes Lebesgue measure on the torus, $\Lambda(b)$.

The proof of Theorem 1 follows from the \hbar -microlocal, regular quantum normal construction near $\Lambda(b)$ (see the section “Birkhoff normal forms”).

Blow-Up of Eigenfunctions: Qualitative Results

Before discussing quantitative bounds for joint eigenfunctions, it is useful to prove qualitative results. Here, we review only the homogeneous case where $P_1 = \hbar \sqrt{\Delta}$, although the general case can be dealt with similarly (Toth and Zelditch 2002). Two well-known QCI examples which exhibit extremes in eigenfunction concentration are the round sphere and the flat torus. In the case of the sphere, the zonal harmonics blow-up like $\lambda^{1/2}$ at the poles, whereas, in the case of the flat torus, all the joint eigenfunctions are uniformly bounded. The rest of the article will be

essentially devoted to understanding these extreme blow-up properties (and intermediate ones) more systematically. When discussing blow-up of eigenfunctions, it is natural to start with the following:

Question Do there exist QCI manifolds (other than the flat torus) for which all eigenfunctions are uniformly bounded in L^∞ ?

Toth and Zelditch (2002) have proved that, up to coverings, the flat torus is the only example with uniformly bounded eigenfunctions. Their argument used the correspondence principle in Theorem 1 combined with some deep results from symplectic geometry. To deal with the issue of multiplicities, it is convenient to define

$$L^\infty(\lambda; g) = \sup_{\varphi \in V_\lambda} \|\varphi\|_{L^\infty}$$

where $V_\lambda = \{\varphi; P_1\varphi = \lambda\varphi\}$ and it is assumed that $\|\varphi\|_{L^2} = 1$.

Theorem 2 (Toth and Zelditch 2002). *Suppose that $P_1 = \sqrt{\Delta}$ is QCI on a compact, Riemannian manifold (M, g) and suppose that the corresponding moment map satisfies the finite-complexity condition. Then, if $L^\infty(\lambda, g) = \mathcal{O}(1)$, (M, g) is flat.*

The proof of Theorem 2 follows by contradiction: that is, one assumes that all eigenfunctions are uniformly bounded. There are two main steps in the proof of Theorem 2: the first is entirely analytic and uses the correspondence principle in Theorem 1 and uniform boundedness to determine the topology of M . The second step uses two deep results from symplectic topology/geometry to determine the metric, g , up to coverings.

Using a local Weyl law argument and the finite-multiplicity assumption, it can be shown that for each $b \in \mathcal{B}_{reg}$, there exists a subsequence, φ_μ , of joint eigenfunctions such that Proposition 1 holds with

$$|c(\hbar; b)|^2 \geq \frac{1}{C}$$

where $C > 0$ is a uniform constant not depending on $b \in \mathcal{B}_{reg}$. With this subsequence, one applies Theorem 1 with $a(x, \xi) = V(x) \in C^\infty(M)$. It then easily follows by the boundedness assumption that for \hbar sufficiently small and appropriate constants $C_0, C_1 > 0$,

$$\begin{aligned} & \left| \int_{\Lambda(b)} (\pi_{\Lambda(b)}^* V) d\mu_b \right| \\ & \leq \frac{1}{C_0} \int_M |V(x)| |\varphi_\mu(x)|^2 d\text{Vol}(x) \\ & \leq \frac{1}{C_1} \int_M |V(x)| d\text{Vol}(x) \end{aligned} \quad [4]$$

where $\pi_{\Lambda(b)}$ denotes the restriction of the canonical projection $\pi: T^*M \rightarrow M$ to the Lagrangian $\Lambda(b)$. The estimate in [4] is equivalent to the statement,

$$(\pi_{\Lambda(b)})_*(d\mu_b) \ll d\text{Vol}(x)$$

where given two Borel measures $d\mu$ and $d\nu$, one writes $d\mu \ll d\nu$ if $d\mu$ is absolutely continuous with respect to $d\nu$. Consequently, $\pi_{\Lambda(b)}: \Lambda(b) \rightarrow M$ has no singularities and thus, up to coverings, M is topologically a torus (since $\Lambda(b)$ is).

Since there are many QCI systems on n -tori, it still remains to determine how the uniform-boundedness condition constrains the metric geometry of (M, g) . First, by a classical result of Mane, if T^*M possesses a C^1 -foliation by Lagrangians, (M, g) cannot have conjugate points. By the first step in the proof, it follows that under the uniform-boundedness assumption, M is a topological torus and T^*M possesses a smooth foliation by Lagrangian tori. Consequently, (M, g) has no conjugate points. Finally, the Burago–Ivanov proof of the Hopf conjecture says that metric tori without conjugate points are flat. Therefore, (M, g) is flat.

Consistent with Theorem 2, one can show (Toth and Zelditch 2003, Lerman and Shirokova 2002) that if (M, g) is integrable and not a flat torus, then there must exist a compact Φ_t -orbit (i.e., an orbit of the joint flow of $X_{p_j}, j = 1, \dots, n$) with $\dim = k < n$. In the QCI case, these “singular” orbits trap eigenfunction mass for appropriate subsequences. To understand this statement in detail, it is necessary to review QBNF constructions in the context of QCI systems.

Birkhoff Normal Forms

There are several excellent expositions on the topic of Birkhoff normal forms in the literature (see, e.g., Guillemin (1996), Iatchenko *et al.* (2002), and Zelditch (1998)), which discuss both the classical and quantum constructions. Here, we discuss the aspects which are most relevant for QCI systems.

Consider the Schrödinger operator, $P(x; \hbar D_x) = -\hbar^2(d^2/dx^2) + V(x)$ with $V(x + 2\pi) = V(x)$ acting on $C^\infty(\mathbb{R}/2\pi\mathbb{Z})$. Assume that the potential, $V(x)$, is Morse and that $x = 0$ is a potential minimum with $V(0) = V'(0) = 0$ and $\Omega \subset T^*(S^1)$ an open neighborhood containing $(0, 0)$. In its simplest incarnation, the classical Birkhoff normal-form theorem says that for small enough Ω , there exists a symplectic diffeomorphism, $\kappa^{-1}: (\Omega; (0, 0)) \rightarrow (\Omega; (0, 0)); \kappa^{-1}: (x, \xi) \mapsto (y, \eta)$, and a (locally defined) function $F_0 \in C^\infty(\mathbb{R})$ such that

$$(p \circ \kappa)(y, \eta) = F_0(\eta^2 + y^2) \quad [5]$$

provided $(y, \eta) \in \Omega$. At the quantum level, the analogous QBNF expansion says that there exist microlocally unitary \hbar -Fourier integral operators, $U(\hbar): C^\infty(\Omega) \rightarrow C^\infty(\Omega)$ and a classical symbol $F(x, \hbar) \sim \sum_{j=0}^{\infty} F_j(x) \hbar^j$, such that

$$U(\hbar)^* \circ P(\hbar) \circ U(\hbar) = {}_\Omega F(\hat{I}_e; \hbar) \quad [6]$$

with $\hat{I}_e = \hbar^2 D_y^2 + y^2$. Given two \hbar -pseudos P and Q , the notation $\hat{P} = {}_\Omega Q$ means that $\|\chi(P - Q)\|_{L^2} = \mathcal{O}(\hbar^\infty)$ and $\|(P - Q)\chi\|_0 = \mathcal{O}(\hbar^\infty)$, for any $\chi \in C_0^\infty(\Omega)$. Since it can be easily shown that eigenfunctions φ_μ , with $\mu(\hbar) = \mathcal{O}(\hbar^\beta)$, $0 < \beta \leq 1$, localize very sharply near $x=0$, from the \hbar -microlocal unitary equivalence in [6], the eigenfunction and eigenvalue asymptotics (including trace formulas) can all be determined by working with the model operator on the right-hand side (RHS) of [6]. Moreover, on the model side, the eigenfunctions and eigenvalues are explicitly known.

At a potential maximum, there exist classical and quantum normal forms analogous to [5] and [6] (see Helffer and Sjostrand (1990) and Colin de Verdiere and Parisse (1994a)) except that the harmonic oscillator action operator, \hat{I}_e , is replaced by the hyperbolic action operator,

$$\hat{I}_h = \hbar(yD_y + \tfrac{1}{2}) \quad [7]$$

The 1D Schrödinger operator is the simplest example of a QCI system where $(0, 0) \in T^*S^1$ is a nondegenerate critical point of the classical Hamiltonian, $H(x, \xi) = \xi^2 + V(x)$. Under a mild nondegeneracy hypothesis (Vu Ngoc 2000), there is an analogous normal form for arbitrary QCI systems which is valid near nondegenerate rank $k < n$ orbits of the joint flow, Φ_t . At the classical level, this result is due to Eliasson (1984) and the quantum analog is due to Vu-Ngoc (2000). To state the result is general, one has to define the appropriate model operators: these are \hat{I}_e and \hat{I}_h together with the loxodromic model operators $\Re \hat{I}_{ch} = \hbar D_\theta$, $\Im \hat{I}_{ch} = \hbar \rho D_\rho + \hbar/i$, where (ρ, θ) denote polar coordinates in \mathbb{R}^2 . The local model phase space for a rank $k < n$ orbit, \mathcal{O}_k , is just $T^*(T^k) \times T^*(\mathbb{R}^{n-k})$. In this case, the QBNF says that, for a sufficiently small neighborhood, \mathcal{G}_k of \mathcal{O}_k , there exists a family of \hbar -Fourier integral operators, $U_\kappa: C^\infty(\mathcal{G}_k) \rightarrow C^\infty(T^*(T^k) \times T^*(\mathbb{R}^{n-k}))$ and symbols $f_j(\hbar) \sim \sum_{j=0}^{\infty} f_j \hbar^j$, such that

$$U_\kappa^* P_j U_\kappa = g_k \mathcal{M}_h \cdot (Q_1 - f_1(\hbar), \dots, Q_n - f_n(\hbar)) \quad [8]$$

$$U_\kappa^* \circ U_\kappa = g_k \text{Id}$$

Here, \mathcal{M}_h is a microlocally invertible matrix of \hbar -pseudodifferential operators commuting with the Q_j 's, and the Q_j 's are to be chosen from the list of model operators $\{\hat{I}_{ch}, \hat{I}_h, \hat{I}_e, \hat{I}_{reg}\}$, where $\hat{I}_{reg} =$

$(\hbar D_{\theta_1}, \dots, \hbar D_{\theta_k})$ denotes the regular model operator acting along the k -dimensional orbit, \mathcal{O}_k . Moreover, if $(y_1, \dots, y_{n-k}, \eta_1, \dots, \eta_{n-k}) \in T^*(\mathbb{R}^{n-k})$ denote the symplectic model coordinates, then the Q_j 's act in separate, complementary (y_1, \dots, y_{n-k}) -variables. The main point here is that [8] is actually a convergent normal form in \hbar in the sense that error terms in [8] are $\mathcal{O}(\hbar^\infty)$. In contrast (Guillemin 1996, Iatchenko *et al.* 2002, Zelditch 1998), the general Birkhoff normal form is only formal in the sense that error terms vanish to successively higher orders along the orbit, \mathcal{O}_k , but are not necessarily small in terms of the spectral parameter, \hbar .

Using [8], it can be shown that the joint eigenfunctions, φ_μ , are microlocally determined in terms of the \hbar -Fourier integral operators, U_κ , and certain model eigenfunctions. More precisely,

$$U_\kappa^* \varphi_\mu(\theta, y; \hbar) = g_k c(\hbar) e^{im\theta} \cdot [u_h \cdot u_{ch} \cdot u_e](y; \hbar) \quad [9]$$

where $m \in \mathbb{Z} + 1/4$, $c(\hbar) \in \mathbb{C}(\hbar)$. The generalized eigenfunctions of the model operators, $\hat{I}_h, \hat{I}_{ch}, \hat{I}_e$, acting transversely to the orbit \mathcal{O}_k are $u_h(y; \mu, \hbar) = c_+(\hbar)|y|^{-1/2+i\mu/\hbar} + c_-(\hbar)|y|^{-1/2-i\mu/\hbar}$, $u_{ch}(\rho, \theta; t, k, \hbar) = \rho^{it/\hbar-1} e^{ik\theta}$ and $u_e(y; n, \hbar) = H_n(\hbar^{-1/2}y)$, where $H_n(y)$ is the n th Hermite function.

Eigenfunction Lower Bounds: Quantitative Results

Let \mathcal{O}_k be a singular rank $k < n$ orbit as in the previous section. From the qualitative results of the first section, it follows that there must exist joint eigenfunctions, φ_μ , of the commuting operators, $P_j, j=1, \dots, n$, which blow up along the orbit, \mathcal{O}_k . To obtain quantitative results, one could try to determine the $L^p \rightarrow L^q$ mapping properties of the \hbar -Fourier integral operator, U_κ . However, since the canonical transformation κ to normal form can be complicated, this method is quite cumbersome. To avoid this complication (Toth and Zelditch 2003), it suffices to compute L^2 -masses only, but on scales of order \hbar^δ where $0 \leq \delta < 1/2$. Let $\pi(\mathcal{G}_k(\hbar^\delta))$ be the configuration space projection of the \hbar^δ -radius tube $\mathcal{G}_k(\hbar^\delta) \supset \mathcal{O}_k$. Since

$$\|\varphi_\mu\|_{L^\infty}^2 \cdot \text{Vol}(\pi(\mathcal{G}_k(\hbar^\delta))) \geq \int_{\mathcal{G}_k(\hbar^\delta)} |\varphi_\mu|^2 d\text{Vol} \quad [10]$$

one is reduced to estimating $\int_{\mathcal{G}_k(\hbar^\delta)} |\phi_\mu|^2 d\text{Vol}$ from below. To bound this integral from below, it suffices to

1. reduce the estimate to one involving only the model eigenfunctions in the Birkhoff normal form and
2. estimate the normalizing \hbar -dependent constant $c(\hbar)$ in [9].

To prove (1) one introduces a cutoff function $\chi(x, \xi; \hbar^\delta) \in C_0^\infty(\mathcal{G}_k(\hbar^\delta))$ and is identically equal to one near \mathcal{O}_k . Then, since $\pi^{-1}(\pi(\mathcal{G}_k(\hbar^\delta))) \supset \mathcal{G}_k(\hbar^\delta)$, from the Garding inequality, it follows that

$$\int_{\mathcal{G}_k(\hbar^\delta)} |\varphi_\mu|^2 d\text{Vol} \gg \langle \text{Op}_\hbar(\chi(x, \xi; \hbar^\delta)) \varphi_\mu, \varphi_\mu \rangle \quad [11]$$

In light of the QBNF result in [8], the computation of the matrix element on the RHS of [11] is reduced to a corresponding computation for the L^2 -normalized model eigenfunctions. Since the U_κ 's are microlocally unitary, it follows that

$$\langle \text{Op}_\hbar(\chi(x, \xi; \hbar^\delta)) \varphi_\mu, \varphi_\mu \rangle \sim_{\hbar \rightarrow 0^+} C(\delta) \cdot |c(\hbar)|^2 \quad [12]$$

Here, the constant $C(\delta) > 0$ depends only on the scale of the cutoff function. It finally remains to deal with (2). Bounding the size of $|c(\hbar)|$ from below amounts to estimating the L^2 -mass of the joint eigenfunction φ_μ which must be trapped near the orbit, \mathcal{O}_k . Using a local (singular) Weyl law argument, it is shown in Toth and Zelditch (2003) that

$$|c(\hbar)|^2 \gg |\log \hbar|^{-\beta} \quad [13]$$

where $\beta > 0$ indexes the number of hyperbolic and loxodromic model operators. The final result quantifies blow-up along a compact orbit:

Theorem 3 (Toth and Zelditch 2003). *Let \mathcal{O}_k be a rank $k < n$ orbit of the joint flow Φ_t . If this orbit is compact and nondegenerate, then there exists a subsequence of L^2 -normalized joint eigenfunctions $\varphi_{\lambda_{j_k}}, k=1, 2, \dots$, of the QCI system $P_j, j=1, \dots, n$, such that for any $\epsilon > 0$,*

$$\|\varphi_{\lambda_{j_k}}\|_{L^\infty} \gg_\epsilon \lambda_{j_k}^{(n-k/4)-\epsilon}$$

By using the semiclassical scale $\hbar^{1/2} |\log \hbar|^{1/2}$, one can (slightly) improve the lower bound in Theorem 3 to $\|\varphi_{\lambda_{j_k}}\|_{L^\infty} \gg_\epsilon \lambda_{j_k}^{n-k/4} |\log \lambda_{j_k}|^{-\alpha}$ for some $\alpha \geq 0$ (see Sogge *et al.* (2005)).

When (M, g) is not flat, there must exist a singular, compact orbit of dimension k with $1 \leq k \leq n-1$ and so, as an immediate corollary of Theorem 3, it follows that for some $\alpha \geq 0$,

$$L^\infty(\lambda; g) \gg \lambda^{1/4} |\log \lambda|^{-\alpha} \quad [14]$$

Since the bound in [14] is highly dependent on dimension, establishing the existence of high-codimension singular orbits would strengthen the estimate substantially. However, this appears to be a difficult and open problem.

Maximal Blow-Up of Modes and Quasimodes

We review here a number of converses to a recent result of Sogge and Zelditch (2002) on Riemannian manifolds (M, g) with maximal eigenfunction growth. These authors proved that if there exists a sequence of L^2 -normalized eigenfunctions of the Laplacian Δ of (M, g) whose L^∞ -norms are comparable to zonal spherical harmonics on S^n , then there must exist a point comparable to the north pole of S^n , that is, a recurrent point z such that a positive measure of geodesics emanating from z return to it at a fixed time T . The most extreme kind of recurrent point is a “blow-down point” of period T , where by definition all geodesics leaving z return to z at time T , that is, form geodesic loops. Poles of surfaces of revolution are blow-down points where all geodesic loops at z are smoothly closed, while umbilic points of triaxial ellipsoids are examples of blow-down points where all but two geodesic loops are not smoothly closed. On real-analytic manifolds, all recurrent points are blow-down points. The converse question is the following: what kind of mode (eigenfunction) or quasimode growth must occur when a blow-down point exists?

Sogge *et al.* (2005) proved that maximal quasimode growth (Colin de Verdière 1977) implies the existence of a blow-down point. This generalizes the main result of Sogge and Zelditch (2002) from modes (which one rarely understands) to quasimodes (which one often understands better). Conversely, existence of a blow-down point insures near-maximal quasimode growth, that is, here, maximal up to logarithmic factors. If one assumes that the geodesic flow $G^t: T^*M \rightarrow T^*M$ of (M, g) is completely integrable and that $\dim M = 2$, then the results of Sogge *et al.* (2005) show that actual eigenfunctions have near maximal blow-up. Examples show that, in general, blow-up points do not necessarily cause modes to have near-maximal blow-up.

An important geometric invariant of a blow-down point is the first-return map to the cotangent fiber over the blow-down point:

$$G_z^T: S_z^*M \rightarrow S_z^*M \quad [15]$$

G_z^T is also an important analytic invariant: the blow-up rate of modes or quasimodes, specifically the occurrence of the logarithmic factors, depends on the fixed-point structure of this map. When all geodesic loops at z are smoothly closed, that is, when the first-return map is the identity, then there exist quasimodes of maximal growth. When the first-return map has fixed points, the maximal growth is modified by logarithmic factors.

To put these results in context, we first recall the local Weyl law of Avakumovich–Levitan (Duistermaat and Guillemin 1975), which states that

$$\sum_{\lambda_\nu \leq \lambda} |\varphi_\nu(x)|^2 = (2\pi)^{-n} \int_{p(x, \xi) \leq \lambda} d\xi + R(\lambda, x) \quad [16]$$

with uniform remainder bounds

$$|R(\lambda, x)| \leq C\lambda^{n-1} \quad x \in M$$

It follows that

$$L^\infty(\lambda, g) = O(\lambda^{(n-1)/2}) \quad [17]$$

on any compact Riemannian manifold. Riemannian manifolds for which the equality

$$L^\infty(\lambda, g) = \Omega(\lambda^{(n-1)/2}) \quad [18]$$

is achieved for some subsequence of eigenfunctions are said to be of maximal eigenfunction growth. In addition to modes, and almost inseparable from them, are the quasimodes of the Laplacian (Colin de Verdière 1977). As the name suggests, quasimodes are approximate eigenfunctions. The crudest type of quasimode is quasimode $\{\psi_k\}$ of order 0, namely a sequence of L^2 -normalized functions which solve

$$\|(\Delta - \mu_k)\psi_k\|_{L^2} = O(1)$$

for a sequence of quasideigenvalues μ_k . By the spectral theorem, it follows that there must exist true eigenvalues in the interval $[\mu_k - \delta, \mu_k + \delta]$ for some $\delta > 0$. (M, g) is said to have maximal 0-order quasimode growth if there exists a sequence of quasimodes of order 0 for which $\|\psi_k\|_{L^\infty} = \Omega(\lambda^{(n-1)/2})$. There are analogous definitions for more refined quasimodes, for example, quasimodes of higher order or (most refined) quasimodes defined by oscillatory integrals. It is natural to include quasimodes in this study because they often reflect the geometry and dynamics of the geodesic flow more strongly than actual modes. For quasimodes, there is the following result:

Theorem 4 (Sogge *et al.* 2005). Let (M^n, g) be a compact Riemannian manifold with Laplacian Δ . Then:

- (i) If there exists a quasimode sequence $\{(\psi_k, \mu_k)\}$ of order 0 with $\|\psi_k\|_{L^\infty} = \Omega(\mu_k^{(n-1)/2})$, then there exists a recurrent point $z \in M$ for the geodesic flow. If (M, g) is real analytic, then there exists a blow-down point.
- (ii) Conversely, if there exists a blow-down point and if the map $G_z^T = \text{id}$, then there exists a quasimode sequence $\{(\psi_k, \mu_k)\}$ of order 0 with $\|\psi_k\|_{L^\infty} = \Omega(\mu_k^{n-1})$.

- (iii) Let $n=2$ and (M^n, g) be real analytic. Then, if G_z^T has a finite number of nondegenerate fixed points, there exists a quasimode sequence $\{(\psi_k, \mu_k)\}$ of order 0 with $\|\psi_k\|_{L^\infty} = \Omega(\mu_k^{1/2} \times |\log \mu_k|^{-1/2})$.

The assumption that $G_z^T = \text{id}$ is the same as saying that all geodesics leaving z smooth close up at z again. As mentioned above, poles of surfaces of revolution have this property. On the contrary, the umbilic points of triaxial ellipsoids in \mathbb{R}^3 are blow-down points for which $G_z^T \neq \text{id}$. That is, every geodesic leaving an umbilic point returns at the same time, but only two closed geodesics in this family are closed, and they give rise to fixed points of G_z^t . One can show (see Toth 1996) that there exists a sequence of eigenfunctions in this case for which $L^\infty(g, \lambda) \sim \lambda^{1/2} |\log \lambda|^{-1/2}$. Hence, the above result is sharp. Moreover, it is clear from the proof that the fixed points are responsible for the logarithmic correction to maximal eigenfunction growth: they cause a change in the normal form of the Laplacian near the blow-down point.

Theorem 4 illustrates the intimate connection between maximal blow-up of quasimodes and existence of blow-down points. It is natural to ask, however, when blow-down points cause blow-up in modes, that is, actual eigenfunctions. As mentioned above, this is not generally the case and some further mechanism is needed to ensure it. In the case of QCI surfaces, one can prove:

Theorem 5 (Sogge *et al.* 2005). Let (M, g) be a smooth, compact surface, $P_1 = \sqrt{\Delta}$, P_2 be an Eliasson nondegenerate QCI system on M and φ_k be an L^2 -normalized joint eigenfunction of P_1, P_2 with $\sqrt{\Delta}\varphi_k = \lambda_k\varphi_k$. Suppose that there exists a blow-down point $z \in M$ for the geodesic flow $G_t := \exp tX_{p_1}$. Then, there exists a subsequence of (joint) Laplace eigenfunctions, $\varphi_{j_k}, k=1, 2, \dots$, such that for any $\epsilon > 0$,

$$\|\varphi_{j_k}\|_{L^\infty} \gg_\epsilon \lambda_{j_k}^{(1/2)-\epsilon}$$

The role of complete integrability is to force joint eigenfunctions to localize on level sets of the moment map and thus to blow up at blow-down points. The proofs of Theorems 4 and 5 are similar. To prove the latter, by the same reasoning as in the orbit case (Theorem 3), one needs to bound from below the integral

$$\int_{B(z, h^\delta)} |\varphi_\mu|^2 d\text{Vol} \quad [19]$$

for an appropriate subsequence of φ_μ s, where $B(z; \hbar^\delta)$ denotes a ball of radius \hbar^δ centered at the blow-down point, $z \in M$. The blow-down condition implies that $S_z^*M \subset \mathcal{P}^{-1}(b)$ for some $b \in \mathcal{B}$. The relevant subsequence of eigenfunctions, φ_μ , are the ones with joint eigenvalues satisfying $|\mu(\hbar) - b| = \mathcal{O}(\hbar)$. Since the eigenfunctions φ_μ are microlocally concentrated on the set $\mathcal{P}^{-1}(b)$, by Gårding,

$$\int_{B(z; \hbar^\delta)} |\varphi_\mu|^2 d\text{Vol} \gg \langle \text{Op}_\hbar(\chi(x, \xi; \hbar^\delta)) \varphi_\mu, \varphi_\mu \rangle \quad [20]$$

where $\chi(x, \xi, \hbar^\delta)$ is a cutoff localized on an \hbar^δ -neighborhood of $\Omega = \pi^{-1}(z) \cap \mathcal{P}^{-1}(b)$. The matrix elements on the RHS of [20] are estimated by passing to QBNF. The subtlety here lies in the choice of scale, δ . For $0 < \delta < 1/2$, the \hbar -pseudodifferential operators $\text{Op}_\hbar(\chi(x, \xi; \hbar^\delta))$ are contained in a standard calculus (Dimassi and Sjostrand 1999) and so they automatically satisfy the \hbar -Egorov theorem. In particular, the passage to normal form by conjugating with the U_κ 's is automatic. The crucial point here is that to obtain the (near)-maximal blow-up near a blow-down point $z \in M$, one needs to be able to choose $0 \leq \delta < 1$. Using second-microlocal methods similar to the ones in Sjostrand and Zworski (1999), it is shown in Sogge *et al.* (2005) that the blow-down geometry implies that the microlocal cutoffs are contained in an \hbar -pseudodifferential operator calculus and, in particular, the relevant \hbar -Egorov theorem needed to pass to QBNF is satisfied for any $0 \leq \delta < 1$. Then, by explicit computation for the model eigenfunctions, one can show that

$$\text{Op}_\hbar(\chi(x, \xi; \hbar^\delta)) \varphi_\mu, \varphi_\mu \gg_\delta \hbar^\delta \quad [21]$$

for any δ with $0 < \delta < 1$. The result in Theorem 5 then follows from the bound

$$\|\varphi_\mu\|_{L^\infty}^2 \cdot \text{Vol}(B(z; \hbar^\infty)) \gg_\delta \hbar^\delta \quad [22]$$

where one takes δ arbitrarily close to 1. By analyzing the U_κ s carefully (Sogge *et al.* 2005), the lower bound in Theorem 5 can be improved slightly by replacing the $\lambda^{-\epsilon}$ by $|\log \lambda|^{-\alpha}$ for some $\alpha > 0$, although the sharp constant, $\alpha > 0$, appears to be difficult to determine in general. In cases where the geometry of the first-return map, G_z^T , is particularly simple, one can sometimes get sharp $|\log \lambda|$ -power improvements in Theorem 5 (see Theorem 4 (iii)).

Eigenfunction Upper Bounds: Quantitative Results

In light of the Ω -bounds in Theorem 5, it is natural to ask whether there are analogous upper bounds for $L^\infty(\lambda; g)$ in the QCI case. The following result holds in the case of real-analytic surfaces:

Theorem 6 (Sogge *et al.* 2005). *Let (M, g) be a real-analytic Riemannian 2-manifold and $P_1 = \sqrt{\Delta}$ and P_2 be a QCI system on (M, g) where, the principal symbol, p_2 , of P_2 is a metric form on T^*M .*

(i) *If $M \cong T^2$,*

$$L^\infty(\lambda; g) = \mathcal{O}(\lambda^{1/4})$$

(ii) *If $M \cong S^2$, let M_{rec} be the set of completely recurrent points for the geodesic flow, $G_t: T^*M \rightarrow T^*M$ and let $\Omega_{\text{rec}} \subset M$ be an open neighborhood of M_{rec} . Then,*

$$L^\infty(\lambda; g)|_{M - \Omega_{\text{rec}}} = \mathcal{O}(\lambda^{1/4})$$

An old result of Kozlov says that if the surface (M, g) is analytic, then topologically either $M \cong S^2$ or $M \cong T^2$, so that the estimates in Theorem 6 cover all possible cases in two dimensions. The assumptions in Theorem 6 are satisfied in many examples including surfaces of revolution, Liouville surfaces, and ellipsoids with distinct axes in \mathbb{R}^3 .

The proof of Theorem 6 follows from a pointwise (joint) trace formula argument (Duistermaat and Guillemin 1975). Namely, in Sogge *et al.* (2005), it is shown that if there are no blow-down points for G_t , then for appropriate $\rho \in \mathcal{S}(R)$ with $\rho \geq 0$ and $\hat{\rho} \in C_0^\infty(R)$,

$$\sum_{j=1}^{\infty} \rho(\hbar^{-1} [\mu_j^{(1)}(\hbar) - b_1]) \cdot \rho(\hbar^{-1} [\mu_j^{(2)}(\hbar) - b_2]) \times |\varphi_\mu(x; \hbar)|^2 = \mathcal{O}(\hbar^{-1/2}) \quad [23]$$

where the estimate in [23] is uniform in $x \in M$ and locally uniform in $b = (b_1, b_2) \in \mathcal{B}$. Part (ii) follows from this. To prove part (i), one applies a simple homological argument to show that if $M \cong T^2$, there cannot exist blow-down points for the geodesic flow (see also Sogge and Zelditch (2002)).

Open Problems

Most questions related to eigenfunction blow-up are completely open and general results are rare (Sogge and Zelditch 2002). Specific results/conjectures in the ergodic case can be found in Quantum Ergodicity and Mixing of Eigenfunctions. We would like to point out here some specific questions related to the above results in the QCI case:

1. All the known examples with blow-down points turn out to be integrable. Is this necessarily always the case?
2. Does the maximal bound $L^\infty(\lambda; g) \sim \lambda^{(n-1)/2}$ necessarily imply that (M, g) is QCI?

3. At the other extreme, does the minimal bound $L^\infty(\lambda; g) \sim 1$ necessarily imply that (M, g) is flat, or do there exist nonflat manifolds (which are necessarily not QCI) satisfying $L^\infty(\lambda; g) \sim 1$?

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See also: Functional Equations and Integrable Systems; Quantum Ergodicity and Mixing of Eigenfunctions.

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Eight Vertex and Hard Hexagon Models

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Introduction

The goal of statistical mechanics is to calculate the macroscopic properties of matter from a knowledge of the fundamental interactions between the constituent microscopic components. For simplicity, let us assume discrete states. The mathematical problem, as formulated by Gibbs, is then to calculate the partition function

$$Z_N = \sum_{\text{states } \sigma} e^{-\beta H(\sigma)} \quad [1]$$

where $\beta = 1/k_B T$ is the inverse temperature, k_B is the Boltzmann constant, and the Hamiltonian H describes the interaction energy of the state σ of the

N constituent degrees of freedom. The formidable nature of the problem ensues from the fact that Z_N is needed in the limit of an arbitrarily large system to obtain the bulk free energy $\psi(T)$ or partition function per site κ in the thermodynamic limit

$$-\beta\psi(T) = \lim_{N \rightarrow \infty} \frac{1}{N} \log Z_N = \log \kappa \quad [2]$$

This limit generally exists because the free energy of a finite system is extensive, that is, it grows proportionally with the system size. Once the bulk free energy is known, the other thermodynamic potentials are obtained, in principle, by taking derivatives with respect to the temperature T and other thermodynamic fields such as the volume V or the external magnetic field h . Phase transitions and the accompanying critical phenomena are associated with singularities of the bulk free energy as a function of the thermodynamic fields. Up until the beginning of the 1970s, there were

only a handful of two-dimensional lattice models that had yielded exact solution, most notably, the Ising model (free-fermion or dimer model), the spherical model, the square ice, and six-vertex models. This situation changed dramatically with Baxter's solution of the eight-vertex and hard-hexagon models. The methods developed by Baxter make it possible to solve an infinite plethora of two-dimensional lattice models. In this article, we compare and contrast the remarkable properties of these two prototypical models that played such a pivotal role in the emergence of the modern theory of Yang–Baxter integrability.

Definition of the Models

Eight-Vertex Model

The eight-vertex model emerged from the study of two-dimensional ferroelectrics. The local degrees of freedom are arrow states $\alpha, \beta, \gamma, \delta = \pm 1$ which live on the edges of the elementary faces of the square lattice and describe the local polarization within the ferroelectric material. Of the 16 possible configurations around a face, the local configurations of an elementary square face are restricted to the eight configurations shown in Figure 1.

The partition function is

$$Z_N = \sum_{\text{arrow states}} \prod_{\text{faces}} W \begin{pmatrix} \gamma & \beta \\ \delta & \alpha \end{pmatrix} \quad [3]$$

where the Boltzmann face weights are given alternative graphical representations as a face or vertex

$$W \begin{pmatrix} \gamma & \beta \\ \delta & \alpha \end{pmatrix} = \begin{array}{c} \gamma \\ \square \\ \alpha \end{array} \quad \beta = \delta \begin{array}{c} \gamma \\ \text{---} \\ \alpha \end{array} \quad [4]$$

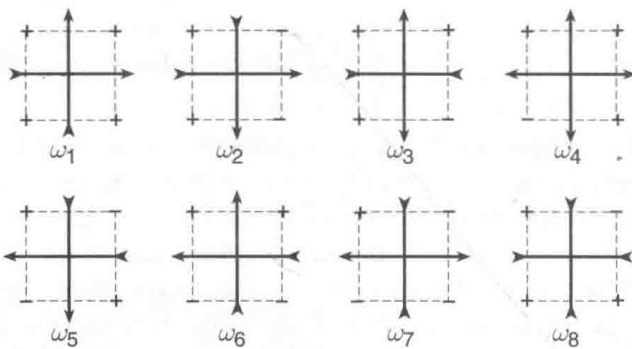


Figure 1 The eight vertex configurations of the eight-vertex model showing one of the two corresponding configurations of the related Ising model. The model is solvable in the symmetric case, $\omega_1 = \omega_5, \omega_2 = \omega_6, \omega_3 = \omega_7, \omega_4 = \omega_8$, when the Boltzmann weights are equal in pairs under arrow reversal.

In the face representation, the arrow states are often called bond variables. Formally, the Hamiltonian is a sum over local energies $H = \sum_{\text{faces}} E(\alpha, \beta, \gamma, \delta)$, where $W(\alpha, \beta, \gamma, \delta) = \exp(-\beta E(\alpha, \beta, \gamma, \delta))$ but we use face weights since E is infinite for excluded configurations. The general eight-vertex model includes many other ferroelectric models including the rectangular Ising model, Slater's model of potassium dihydrogen phosphate (KDP), the Rys F model of an antiferroelectric, the square ice model and the six-vertex model solved by Lieb. In the case of the six-vertex model, $\omega_4 = \omega_8 = 0$, so arrows are conserved with "two in" and "two out" at each vertex.

The eight-vertex model can be formulated as an Ising model with spins $a, b, c, d = \pm 1$ at the corners of the elementary faces and Boltzmann face weights

$$W \begin{pmatrix} d & c \\ a & b \end{pmatrix} = R \exp(Kac + Lbd + Mabcd) \\ = \begin{array}{c} d \quad c \\ \square \\ a \quad b \end{array} = \begin{array}{c} d \\ \diagup \quad \diagdown \\ a \quad b \end{array} \quad [5]$$

The four independent vertex weights are related to R, K, L, M by

$$\begin{aligned} \omega_1 &= \omega_5 = R e^{K+L+M} \\ \omega_2 &= \omega_6 = R e^{-K-L+M} \\ \omega_3 &= \omega_7 = R e^{K-L-M} \\ \omega_4 &= \omega_8 = R e^{-K+L-M} \end{aligned} \quad [6]$$

This is not the usual rectangular Ising model since it involves four-spin interactions in addition to two-spin interactions. The spins and arrows are related by

$$\alpha = ab, \quad \beta = bc, \quad \gamma = cd, \quad \delta = da \quad [7]$$

This mapping is one-to-two, since we can arbitrarily fix one spin somewhere on the lattice. It follows that $Z_{\text{Ising}} = 2Z_{\text{vertex}}$. The eight-vertex model obviously includes the six-vertex ($\omega_4 = \omega_8$) and the rectangular Ising models ($M=0$). Although it is not at all obvious, the three-spin Ising model is also included as a special case ($K=M, L=0$).

Notice that the eight-vertex face weights are invariant under spin reversal of the spins on either diagonal. This $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry, which the eight-vertex model shares with the Ashkin–Teller model, is peculiar because it allows the model to exhibit continuously varying critical exponents. Because of symmetries and duality, it is sufficient to consider the regime $\omega_1 > \omega_2 + \omega_3 + \omega_4$ with $\omega_2, \omega_3, \omega_4 > 0$. In terms of spins, this corresponds to the

ferromagnetically ordered phase; in terms of vertices or arrows, this corresponds to the ferroelectric phase. The eight-vertex model is critical on the four surfaces

$$\begin{aligned} \omega_1 &= \omega_2 + \omega_3 + \omega_4, & \omega_2 &= \omega_1 + \omega_3 + \omega_4 \\ \omega_3 &= \omega_1 + \omega_2 + \omega_4, & \omega_4 &= \omega_1 + \omega_2 + \omega_3 \end{aligned} \quad [8]$$

A convenient parameter to measure the departure from criticality $t = (T - T_c)/T_c$ is

$$t = -\frac{1}{16\omega_1\omega_2\omega_3\omega_4} [(\omega_1 - \omega_2 - \omega_3 - \omega_4) \times (\omega_1 - \omega_2 + \omega_3 + \omega_4) \times (\omega_1 + \omega_2 - \omega_3 + \omega_4) \times (\omega_1 + \omega_2 + \omega_3 - \omega_4)] \quad [9]$$

Because of the unusual four-spin interaction, it is difficult to realize the eight-vertex model experimentally in the laboratory.

Hard-Hexagon Model

The hard-hexagon model is a two-dimensional lattice model of a gas of hard nonoverlapping particles. The particles are placed on the sites of a triangular lattice with nearest-neighbor exclusion so that no two particles are together or adjacent. Effectively, the triangular lattice is partially covered with nonoverlapping hard tiles of hexagonal shape. Let us draw the triangular lattice as a square lattice with one set of diagonals as in Figure 2. The partition function for the hard-hexagon model is

$$Z_N = \sum_{n=0}^N z^n g(n, N) \quad [10]$$

where $z > 0$ is the activity and $g(n, N)$ is the number of ways of placing n particles on the N sites such that no two particles are together or adjacent. To each lattice site j , assign a spin or occupation

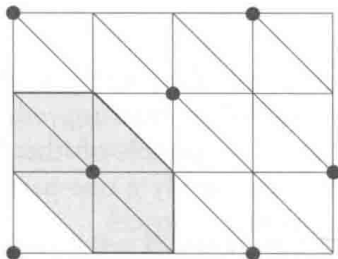


Figure 2 The triangular lattice drawn as a square lattice with one set of diagonals. The close-packed arrangement of particles (solid circles) fills one of the three independent sublattices. One of the nonoverlapping hard hexagons is shown shaded. At low activities, the hard hexagons are sparsely scattered on the lattice with no preferential occupation of a particular sublattice.

number σ_j ; if the site is empty, $\sigma_j = 0$; if the site is full, $\sigma_j = 1$. The partition function can then be written in terms of spins as

$$Z_N = \sum_{\text{spins } \sigma} \prod_{\langle ij \rangle} z^{(\sigma_i + \sigma_j)/6} (1 - \sigma_i \sigma_j) \quad [11]$$

where the product is over all bonds $\langle ij \rangle$ of the triangular lattice and the sum is over all configurations of the N spins or occupation numbers $\sigma_j = 0, 1$. The exponent of z arises because the activity is shared out between the six bonds incident at each site. The remaining term, $(1 - \sigma_i \sigma_j) = 0, 1$, ensures that neighboring sites are not occupied simultaneously by excluding such terms from the sum.

The activity z gives the *a priori* probability of finding a particle at a given site and can be written as $z = e^{-\beta\mu}$, where μ is the chemical potential. The density of particles increases monotonically as the activity increases but only a third of the total lattice sites can be occupied. At low activities, there are only a few particles scattered randomly so the S_3 sublattice symmetry of the triangular lattice is preserved. However, at higher activities approaching the close-packing limit, there is a sudden change and one of the three sublattices is preferentially occupied so the S_3 sublattice symmetry is spontaneously broken. This dramatic change signals an order-disorder phase transition at some critical value z_c of the activity. The system is disordered below the critical activity but is ordered above it. The fundamental problem is to obtain the statistical properties of this model such as the bulk free energy and the sublattice densities

$$\begin{aligned} \rho_k &= \langle \sigma_k \rangle \\ &= \{\text{fraction of spins sitting on} \\ &\quad \text{sublattice } k = 1, 2, 3\} \end{aligned} \quad [12]$$

in the thermodynamic limit $N \rightarrow \infty$. The mean density is

$$\rho = (\rho_1 + \rho_2 + \rho_3)/3 \leq 1/3 \quad [13]$$

Assuming that sublattice $k=1$ is preferentially occupied, an order parameter is defined by

$$R = \rho_1 - \rho_2 \quad [14]$$

The order parameter vanishes in the disordered regime but is nonzero in an ordered regime. Notice that the symmetry between sublattices $k=2$ and 3 is not broken.

Unlike the eight-vertex model, the hard-hexagon model can be realized by a physical system in the laboratory, namely helium adsorbed on a graphite surface. The graphite substrate is composed of hexagonal cells formed by six carbon atoms with

an interatom distance of 2.46 Å. Energetically, the adsorbed helium atoms prefer to sit in the potential well at the center of the hexagonal cells. The diameter of the helium atom, however, is 2.56 Å, which precludes the simultaneous occupation of neighboring cells by excluded volume effects. Some beautiful experiments carried out by Bretz indicate that this system undergoes a phase transition. Indeed, Bretz took precise measurements of the specific heat as the temperature or, equivalently, the activity z , is varied, and obtained a symmetric power-law divergence at the critical point

$$C \sim |z - z_c|^{-\alpha}, \quad \alpha \approx 0.36 \quad [15]$$

with critical exponent α close to 1/3. Of course, one does not actually see divergences experimentally. Rather, it is the presence of dramatic peaks in the specific heat that are the hallmarks of a second-order transition.

Yang-Baxter Equations and Commuting Transfer Matrices

Yang-Baxter Equations

The eight-vertex and hard-hexagon models were solved by Rodney Baxter at the beginning of the 1970s and 1980s, respectively. Although the two models are quite different in nature, they are quintessential of exactly solvable lattice models. The seminal work of Baxter gives a precise criterion to decide if a two-dimensional lattice model is exactly solvable: it is exactly solvable if its local face weights satisfy the celebrated Yang-Baxter equation. We present a general formulation of the Yang-Baxter equations and commuting transfer matrices and then show how Baxter implemented these for the eight-vertex and hard-hexagon models.

The first important step in the exact solution of a two-dimensional lattice model is the parametrization of the Boltzmann weights in terms of a distinguished variable u called the spectral parameter. Typically, critical models involve trigonometric or hyperbolic functions and off-critical models involve elliptic functions of the spectral parameter. In terms of u , the local Boltzmann weights of a general two-dimensional lattice model take the form

$$W \left(\begin{array}{ccc|c} d & \gamma & c & \\ \delta & & \beta & u \\ a & \alpha & b & \end{array} \right) = \delta \begin{array}{|c|} \hline u \\ \hline \end{array} \beta \quad [16]$$

where the allowed values of the spins a, b, c, \dots and arrows (or bond variables) $\alpha, \beta, \gamma, \dots$ may be

restricted by certain constraints. The spins a, b, c, d are absent for the eight-vertex model and the arrows $\alpha, \beta, \gamma, \delta$ are absent for the hard-hexagon model.

The general Yang-Baxter equations take the following algebraic and graphical forms:

$$\sum_{g, \eta, \xi, \zeta} W \left(\begin{array}{ccc|c} f & \zeta & g & \\ \mu & & \eta & u \\ a & \alpha & b & \end{array} \right) W \left(\begin{array}{ccc|c} e & \delta & d & \\ \epsilon & & \xi & v \\ f & \zeta & g & \end{array} \right) W \left(\begin{array}{ccc|c} d & \gamma & c & \\ \xi & & \beta & v-u \\ g & \eta & b & \end{array} \right) \\ = \sum_{g, \eta, \xi, \zeta} W \left(\begin{array}{ccc|c} e & \eta & g & \\ \epsilon & & \xi & v-u \\ f & \mu & a & \end{array} \right) W \left(\begin{array}{ccc|c} g & \zeta & c & \\ \xi & & \beta & v \\ a & \alpha & b & \end{array} \right) W \left(\begin{array}{ccc|c} e & \delta & d & \\ \eta & & \gamma & u \\ g & \zeta & c & \end{array} \right) \\ \begin{array}{c} \begin{array}{c} e \quad \delta \quad d \\ \epsilon \quad v \quad \gamma \\ f \quad \mu \quad u \\ a \quad \alpha \quad b \end{array} \\ \begin{array}{c} e \quad \delta \quad d \\ \epsilon \quad v-u \quad \gamma \\ f \quad \mu \quad v \\ a \quad \alpha \quad b \end{array} \end{array} = \begin{array}{c} \begin{array}{c} e \quad \delta \quad d \\ \epsilon \quad u \quad \gamma \\ f \quad v-u \quad c \\ a \quad \alpha \quad b \end{array} \\ \begin{array}{c} e \quad \delta \quad d \\ \epsilon \quad v \quad \gamma \\ f \quad \mu \quad v \\ a \quad \alpha \quad b \end{array} \end{array} \quad [17]$$

Graphically, this equation can be interpreted as saying that the diamond-shaped face with spectral parameter $v - u$ can be pushed through from the right to the left with the effect of interchanging the spectral parameters u and v in the remaining two faces.

Commuting Transfer Matrices

A square lattice is built up row-by-row using the row transfer matrix $T(u)$ with matrix elements

$$\langle a, \alpha | T(u) | c, \gamma \rangle = \sum_{\beta_1, \beta_2, \dots, \beta_N = \pm 1} \prod_{j=1}^N W \left(\begin{array}{ccc|c} c_j & \gamma_j & c_{j+1} & \\ \beta_j & & \beta_{j+1} & u \\ a_j & \alpha_j & a_{j+1} & \end{array} \right) \quad [18]$$

$$= \beta_1 \begin{array}{|cccccc|} \hline u & u & u & u & u & u \\ \hline \end{array} \beta_1 \quad [19]$$

$a_1 \alpha_1 \quad a_2 \alpha_2 \quad a_3 \alpha_3 \quad a_4 \alpha_4 \quad \dots \quad a_N \alpha_1 a_1$

Here there are N columns, and periodic boundary conditions are applied so that $a_{N+1} = a_1, \beta_{N+1} = \beta_1$, and so on. The significance of the Yang-Baxter equations is that they imply a one-parameter family of commuting transfer matrices

$$T(u)T(v) = T(v)T(u) \quad [20]$$

Pictorially, the product on the left is represented by two rows, one above the other, the lower row with spectral parameter u and the upper row with spectral parameter v . The matrix product implies

that the spins and arrows on the intervening row are summed out. Inserting a diamond-shaped face with spectral parameter $\nu - u$ and then using the local Yang–Baxter equation to progressively push it from right to left around the period interchanges all of the spectral parameters u with the spectral parameter ν . At the end, the diamond-shaped face is removed again. This heuristic argument was made rigorous by Baxter, who showed quite generally, and for the eight-vertex and hard-hexagon models in particular, that the diamond faces are in fact invertible:

$$\sum_{g, \epsilon, \mu} a \begin{array}{c} \delta \\ \swarrow \quad \searrow \\ u \quad g \\ \swarrow \quad \searrow \\ \alpha \quad \epsilon \quad \epsilon \quad \beta \\ b \quad \quad b \end{array} \begin{array}{c} d \quad \mu \quad d \\ \swarrow \quad \searrow \\ -u \quad c \\ \swarrow \quad \searrow \\ \gamma \quad \delta \end{array} = \rho(u) \delta(a, c) \delta(\alpha, \beta) \delta(\gamma, \delta) \quad [21]$$

independent of b, d where the scalar function $\rho(u)$ is model dependent. This equation is called the inversion relation.

Invariably, the existence of commuting transfer matrices leads to functional equations satisfied by the transfer matrices. Typically, the transfer matrices can be simultaneously diagonalized and so the functional equations can be solved for the eigenvalues of the transfer matrices. Mathematically, this is where Yang–Baxter techniques derive their power. For example, building up the lattice row-by-row, we see that the partition function of an $M \times N$ lattice is

$$Z_{MN} = \text{tr } T(u)^M = \sum_n T_n(u)^M \quad [22]$$

where $T_n(u)$ are the eigenvalues of $T(u)$. Typically, by the Perron–Frobenius theorem, the largest eigenvalue $T_0(u)$ is real, positive, and nondegenerate:

$$T_0(u) > |T_1(u)| \geq |T_2(u)| \geq \dots \quad [23]$$

Consequently,

$$\begin{aligned} -\beta\psi &= \lim_{N \rightarrow \infty} \lim_{M \rightarrow \infty} \frac{1}{MN} \log \sum_n T_n(u)^M \\ &= \lim_{N \rightarrow \infty} \frac{1}{N} \log T_0(u) \end{aligned} \quad [24]$$

Thus the calculation of the bulk free energy is reduced to the problem of finding the largest eigenvalue of the transfer matrix.

Parametrization of the Eight-Vertex Model

Using the spin formulation of the eight-vertex model, Baxter showed that two transfer matrices $T(K, L, M), T(K', L', M')$ commute whenever

$$\Delta(K, L, M) = \Delta(K', L', M') \quad [25]$$

where

$$\Delta(K, L, M) = \sinh 2K \sinh 2L + \tanh 2M \cosh 2K \cosh 2L \quad [26]$$

If M and Δ are regarded as fixed, this is seen to be a symmetric biquadratic relation between e^{2K} and e^{2L} and is naturally parametrized in terms of elliptic functions. Unfortunately, many different notations and conventions for these elliptic functions appear in the literature which can be confusing to the uninitiated. Let

$$s = \frac{\vartheta_1(u)}{\vartheta_1(\lambda)}, \quad s_{\pm} = \frac{\vartheta_1(\lambda \pm u)}{\vartheta_1(\lambda)}, \quad \eta = \frac{\vartheta_1^2(\lambda)}{\vartheta_4^2(\lambda)} \quad [27]$$

$$c = \frac{\vartheta_4(u)}{\vartheta_4(\lambda)}, \quad c_{\pm} = \frac{\vartheta_4(\lambda \pm u)}{\vartheta_4(\lambda)}, \quad \mu = \frac{\vartheta_4(0)}{\vartheta_4(\lambda)} \quad [28]$$

where $\vartheta_1(u) = \vartheta_1(u, q)$ and $\vartheta_4(u) = \vartheta_4(u, q)$ are standard elliptic theta functions of nome q . Then the vertex weights can be parametrized as

$$\begin{aligned} \omega_1 &= R\mu^{-1}cc_{-}, & \omega_2 &= R\eta\mu^{-1}ss_{-} \\ \omega_3 &= R\mu^{-1}cs_{-}, & \omega_4 &= R\mu^{-1}c_{-}s \end{aligned} \quad [29]$$

In the ferromagnetic regime u, λ , and τ are all pure imaginary with $0 < q < 1$ and $0 < \text{Im } u < \text{Im } \lambda < (\pi/2)\text{Im } \tau$. The critical line occurs in the limit $q \rightarrow 1$. In this sense, we are using a low-temperature elliptic parametrization. Another elliptic parametrization, which is useful to study the critical limit, is obtained by transforming to the conjugate nome q' : If $q = e^{-\pi\epsilon}$ then the conjugate nome is defined by $q' = e^{-\pi/\epsilon}$ so that $q' \rightarrow 0$ as $q \rightarrow 1$.

We regard the crossing parameter λ as constant, u as a variable, and write the transfer matrix as $T(u)$. It follows from this parametrization that M and Δ are constants, independent of u . Furthermore, any two transfer matrices $T(u)$ and $T(v)$ commute and hence $T(u)$ is a one-parameter family of commuting transfer matrices. For interest, we point out that the integrable XYZ quantum spin chain belongs to this family. Specifically, the logarithmic derivative of the eight-vertex transfer matrix yields

$$\frac{d}{du} [\log T(u)]_{u=0} = H_{XYZ} \quad [30]$$

where

$$\begin{aligned} H_{XYZ} &= -\frac{1}{2} \sum_{j=1}^N \left(J_x \sigma_j^x \sigma_{j+1}^x + J_y \sigma_j^y \sigma_{j+1}^y + J_z \sigma_j^z \sigma_{j+1}^z \right) \end{aligned} \quad [31]$$

and $\sigma_j^x, \sigma_j^y, \sigma_j^z$ are the usual Pauli spin matrices.

Parametrization of the Hard-Hexagon Model

Actually, Baxter did not solve the hard-hexagon model directly. Instead, he solved a generalized hard-hexagon model, which is a model of hard squares with interactions along the diagonals of the elementary squares as shown in Figure 3. This in turn corresponds to the A_4 case of the more general solvable A_L restricted solid-on-solid (RSOS) models of Andrews, Baxter, and Forrester.

The face weights of the generalized hard-hexagon model are

$$W\begin{pmatrix} d & c \\ a & b \end{pmatrix} = mz^{(a+b+c+d)/4} t^{-a+b-c+d} (1-ab) \\ \times (1-bc)(1-cd)(1-da) \\ \times \exp(Lac + Mbd) \quad [32]$$

Here the activity z has been shared out between the four faces adjacent to a site, m is a trivial normalization constant, and t is a gauge parameter that cancels out of the partition function and transfer matrix. The anisotropy between L and M introduces an additional parameter which will play the role of the spectral parameter u . In fact, using the Yang–Baxter equation, Baxter showed that this model is exactly solvable on the manifold

$$z = (1 - e^{-L})(1 - e^{-M}) / (e^{L+M} - e^L - e^M) \quad [33]$$

Specifically, two transfer matrices $T(z, L, M)$ and $T(z', L', M')$ commute whenever

$$\Delta(z, L, M) = \Delta(z', L', M') \\ \Delta(z, L, M) = z^{-1/2} (1 - ze^{L+M}) \quad [34]$$

The hard-hexagon model is recovered in the limit $L=0, M=-\infty$ which forbids simultaneous occupation of sites joined by one set of diagonals. In this special limit, the activity z is unconstrained. It is curious to note that the pure hard-square model with $L=M=0$ is not solvable.

Eliminating z between the above relations gives a symmetric biquadratic relation between e^L and e^M ,

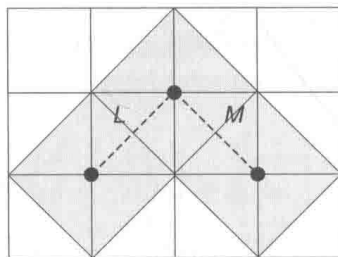


Figure 3 Interacting hard squares showing the diagonal interactions L and M . The hard-hexagon model corresponds to the limit $L=0, M=-\infty$.

which is naturally parametrized in terms of elliptic functions. Choosing m and t appropriately, the Boltzmann weights are

$$W\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} = \frac{\theta(2\lambda + u)}{\theta(2\lambda)} \\ W\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = W\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \frac{\theta(u)}{[\theta(\lambda)\theta(2\lambda)]^{1/2}} \\ W\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = W\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \frac{\theta(\lambda - u)}{\theta(\lambda)} \quad [35] \\ W\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\theta(2\lambda - u)}{\theta(2\lambda)} \\ W\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{\theta(\lambda + u)}{\theta(\lambda)}$$

Here the crossing parameter is $\lambda = \pi/5$, $-\lambda < u < 2\lambda$, and

$$\theta(u) = \theta(u, q^2) \\ = \sin u \prod_{n=1}^{\infty} (1 - q^{2n} e^{2iu}) \\ \times (1 - q^{2n} e^{-2iu})(1 - q^{2n}) \quad [36]$$

is a nonstandard elliptic theta function of nome q^2 . Despite the deceiving notation, the nome q^2 lies in the range $-1 < q^2 < 1$ and is determined by the relation

$$\Delta^2 = \left[\frac{\theta(\lambda)}{\theta(2\lambda)} \right]^5 = z(1 - ze^{L+M})^2 \quad [37]$$

Regarding q^2 as fixed and u as a variable, it follows that $T(u)$ is a one-parameter family of commuting transfer matrices.

The regimes relevant to the hard-hexagon model are:

$$\begin{aligned} \text{Regime I (disordered):} & \quad -1 < q^2 < 0, \\ & \quad -\lambda < u < 0 \\ \text{Regime II (triangular ordered):} & \quad 0 < q^2 < 1, \\ & \quad -\lambda < u < 0 \end{aligned} \quad [38]$$

The borderline case $q^2=0$ corresponds to a line of critical points. The original hard-hexagon model is obtained in the limit $u \rightarrow -\lambda = -\pi/5$, so it follows that the critical point occurs at

$$z_c = \left(\frac{1 + \sqrt{5}}{2} \right)^5 = \frac{1}{2} (11 + 5\sqrt{5}) \quad [39]$$

Away from criticality the activity is related to the nome q^2 by

$$z = z_c \prod_{n=1}^{\infty} \left[\frac{1 - 2q^{2n} \cos(4\pi/5) + q^{4n}}{1 - 2q^{2n} \cos(2\pi/5) + q^{4n}} \right]^5 \quad [40]$$

Functional Equations

Baxter's T - Q Relation

In a *tour de force* Baxter showed that the transfer matrix of the eight-vertex model satisfies the functional equation

$$T(u)Q(u) = \phi(u)Q(u - \lambda) + \phi(u - \lambda)Q(u + \lambda) \quad [41]$$

where $\phi(u) = (cs)^N = [\vartheta_1(u)\vartheta_4(u)/\vartheta_1(\lambda)\vartheta_4(\lambda)]^N$ and $Q(u)$ is an auxiliary family of mutually commuting transfer matrices satisfying $[Q(u), Q(v)] = [Q(u), T(v)] = 0$. In principle, these equations, which are intimately related to the Bethe ansatz, can be solved to obtain all the eigenvalues of the transfer matrix. Without entering into the intricacies of solving these equations, we summarize the results for the partition function per site κ , correlation length ξ , and interfacial tension σ . As we have seen, the largest eigenvalue of the transfer matrix yields κ . The interfacial tension σ and correlation length ξ were obtained, respectively, by Baxter and by Johnson, Krinsky, and McCoy by integrating over (continuous) bands of eigenvalues. In the ferromagnetic regime, their results are

$$\log(\kappa/\omega_1) = \sum_{n=1}^{\infty} \frac{x^{-n}(x^{2n} - q^n)^2(x^n + x^{-n} - z^n - z^{-n})}{n(1 - q^{2n})(1 + x^{2n})} \quad [42]$$

$$\xi^{-1} = -\frac{1}{2} \log k(x^2), \quad \sigma = k_B T / \xi \quad [43]$$

where $x = e^{\pi i \lambda / 2}$, $z = x^{-1} e^{\pi i u}$, and k is the elliptic modulus of nome x^2 :

$$k(x^2) = 4x \prod_{n=1}^{\infty} \left(\frac{1 + x^{4n}}{1 + x^{4n-2}} \right)^4 \quad [44]$$

Detailed analysis shows that near T_c the free energy ψ in general behaves as

$$\psi \sim \cot(\pi^2/2\bar{\mu}) t^{\pi/\bar{\mu}} \sim t^{2-\alpha}, \quad t \rightarrow 0 \quad [45]$$

where $t = (T - T_c)/T_c$,

$$\tan(\bar{\mu}/2) = (\omega_3 \omega_4 / \omega_1 \omega_2)^{1/2} = e^{-2M} \quad [46]$$

and $\alpha = 2 - \pi/\bar{\mu}$ with $0 < \bar{\mu} < \pi$. Exceptional cases occur, however, if $\pi/\bar{\mu}$ is an integer. This occurs, for example, in the case of the rectangular Ising model ($M=0$, $\bar{\mu} = \pi/2$), which exhibits a logarithmic singularity in the specific heat ($\alpha = 0_{\log}$). Similarly, using $\log k(x^2) \sim (-t)^{\pi/2\bar{\mu}}$, the other associated critical exponents are

$$\xi^{-1} \sim (-t)^{\nu}, \quad \sigma \sim (-t)^{\mu}, \quad \nu = \mu = \pi/2\bar{\mu} \quad [47]$$

Notice that, due to the special symmetries of the eight-vertex model, these critical exponents vary continuously as the four-spin interaction is varied. This violates the universality hypothesis, which asserts that the exponents should only depend on the dimensionality and symmetries and not on the details of the interactions. Suzuki has suggested that it is more natural to use the inverse correlation length ξ^{-1} , rather than the temperature difference $T - T_c$, to measure the departure from criticality with the effect that it is the renormalized critical exponents

$$\hat{\alpha} = (2 - \alpha)/\nu, \quad \hat{\beta} = \beta/\nu, \quad \hat{\mu} = \mu/\nu \quad [48]$$

that are independent of the details of the interactions.

Hard-Hexagon Functional Equation

Baxter and Pearce showed that the normalized row transfer matrix of the generalized hard-hexagon model,

$$t(u) = \left[\frac{\theta(u + 2\lambda)\theta(\lambda)}{\theta(u + \lambda)\theta(u - 2\lambda)} \right]^N T(u) \quad [49]$$

satisfies the simple functional equation

$$t(u)t(u + \lambda) = I + t(u - 2\lambda) \quad [50]$$

where $\lambda = \pi/5$. Since $T(u)$ is a commuting family of matrices, this equation can be solved for the eigenvalues $T(u)$ to obtain the partition function per site κ , correlation length ξ , and interfacial tension σ . Let $p = |q^2|$, $s = |q^2|^{5/6}$, then the results are summarized as

$$\kappa = \begin{cases} \kappa_c \prod_{n=1}^{\infty} \frac{[1 - 2q^{2n} \cos(4\pi/5) + q^{4n}]^2 (1 - q^{2n})^2 (1 - p^{5n}) (1 - p^{10(2n-1)/3})^3}{[1 - 2q^{2n} \cos(2\pi/5) + q^{4n}]^3 (1 - p^{5n/3})^3 (1 - p^{10(2n-1)})}, & z \leq z_c \\ \kappa_c \prod_{n=1}^{\infty} \frac{[1 - 2q^{2n} \cos(4\pi/5) + q^{4n}]^2 (1 - q^{2n})^2 (1 - p^{5n})}{[1 - 2q^{2n} \cos(2\pi/5) + q^{4n}]^3 (1 - p^{5n/3})^3}, & z > z_c \end{cases} \quad [51]$$

$$\kappa_c = \left[\frac{27(25 + 11\sqrt{5})}{250} \right]^{1/2} \quad [52]$$

$$e^{-\xi^{-1}} = \begin{cases} \prod_{n=1}^{\infty} \frac{1 - \sqrt{3}s^{2n-1} + s^{4n-2}}{1 + \sqrt{3}s^{2n-1} + s^{4n-2}}, & z \leq z_c \\ \min_{0 < \alpha < \pi} \left[\prod_{n=1}^{\infty} \frac{1 - 2s^{2n-1} \cos(\frac{2\pi}{3} - \alpha) + s^{4n-2}}{1 - 2s^{2n-1} \cos(\frac{2\pi}{3} + \alpha) + s^{4n-2}} \right]^2, & z > z_c \end{cases} \quad [53]$$

$$\sigma = \begin{cases} 0, & z \leq z_c \\ \frac{1}{2} k_B T / \xi, & z > z_c \end{cases} \quad [54]$$

It follows that $\kappa(z)$, $\xi(z)$, and $\sigma(z)$ are analytic functions of z , except at the critical point $z = z_c$.

The associated critical exponents

$$\begin{aligned} \psi &\sim (z - z_c)^{2-\alpha}, & \xi &\sim (z - z_c)^{-\nu} \\ \sigma &\sim (z - z_c)^{-\mu}, & \alpha = 1/3, \quad \nu = \mu = 5/6 \end{aligned} \quad [55]$$

agree with experiments on helium adsorbed on graphite.

Corner Transfer Matrices

The one-point functions and order parameters of the eight-vertex and hard-hexagon models were obtained by Baxter by using corner transfer matrices (CTMs). The idea is to build up the square lattice quadrant-by-quadrant as shown in Figure 4. The partition function and one-point function are then

$$Z = \text{tr } ABCD, \quad \langle \sigma_1 \rangle = \frac{\text{tr } SABCD}{\text{tr } ABCD} \quad [56]$$

where S is the diagonal matrix with entries $S_{\sigma, \sigma} = \sigma_0$ and the entries $A_{\sigma, \sigma'}$ are labeled by half-rows of spins $\sigma = (\sigma_0, \sigma_1, \sigma_2, \dots)$ and $\sigma' = (\sigma_0, \sigma'_1, \sigma'_2, \dots)$.

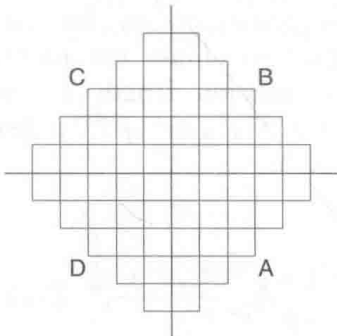


Figure 4 The square lattice divided into four quadrants corresponding to the CTMs **A**, **B**, **C**, **D**. The spin at the center is σ_0 . The spins on the boundaries are fixed by the boundary conditions.

The CTMs have some remarkable properties. If the Boltzmann weights are invariant under reflections about the diagonals, as is the case for the eight-vertex model, Baxter argued that, in the limit of a large lattice,

$$A(u) = C(u) = B(\lambda - u) = D(\lambda - u) \quad [57]$$

where $A(u)$ is a commuting family of matrices. Since these are block matrices in the center spin σ_0 , they also commute with S . Moreover, Baxter showed that the eigenvalues of $A(u)$ are exponentials of the form

$$A(u)_\sigma = m_\sigma \exp(u E_\sigma) \quad [58]$$

where the constants m_σ and E_σ can be evaluated in the low-temperature limit. It follows that

$$\langle \sigma_0 \rangle = \frac{\sum_\sigma \sigma_0 m_\sigma^4 e^{2\lambda E_\sigma}}{\sum_\sigma m_\sigma^4 e^{2\lambda E_\sigma}} \quad [59]$$

When the Boltzmann weights do not exhibit symmetry about the diagonals, which is the case for hard hexagons, the above arguments need to be modified.

One-Point Functions of the Eight-Vertex Model

For the eight-vertex model, Baxter showed that

$$\begin{aligned} m_\sigma &= 1, \quad E_\sigma = \frac{1}{2} \pi i \sum_{j=1}^N j H(\sigma_{j-1}, \sigma_j, \sigma_{j+1}) \\ H(\sigma_{j-1}, \sigma_j, \sigma_{j+1}) &= 1 - \sigma_{j-1} \sigma_{j+1} \end{aligned} \quad [60]$$

subject to the boundary condition $\sigma_N = \sigma_{N+1} = +1$. Introducing a new set of spins

$$\mu_j = \sigma_{j-1} \sigma_{j+1}, \quad j = 1, 2, \dots, N \quad [61]$$

we have $\sigma_0 = \mu_1 \mu_3 \mu_5 \dots$. Setting $s = (xz)^{1/2} = e^{\pi i u/2}$, $t = (x/z)^{1/2} = e^{\pi i (\lambda - u)/2}$ and taking the limit of large N , the diagonalized matrices are direct products of 2×2 matrices:

$$S = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \dots \quad [62]$$

$$\begin{aligned} A(u) &= C(u) \\ &= \begin{pmatrix} 1 & 0 \\ 0 & s \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & s^2 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & s^3 \end{pmatrix} \otimes \dots \end{aligned} \quad [63]$$

$$\begin{aligned} B(u) &= D(u) \\ &= \begin{pmatrix} 1 & 0 \\ 0 & t \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & t^2 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & t^3 \end{pmatrix} \otimes \dots \end{aligned} \quad [64]$$

It follows that the magnetization is

$$\langle \sigma_0 \rangle = \prod_{n=1}^{\infty} \frac{1 - x^{4n-2}}{1 + x^{4n+2}} = (k')^{1/4} = (1 - k^2)^{1/8} \quad [65]$$

where $k' = k'(x^2)$ is the conjugate elliptic modulus of nome x^2 and the associated critical exponent is

$$\langle \sigma_0 \rangle \sim (-t)^\beta, \quad \beta = \pi/16\bar{\mu} \quad [66]$$

The polarization of the eight-vertex model is

$$\langle \alpha \rangle = \langle \sigma_0 \sigma_1 \rangle = \prod_{n=1}^{\infty} \left(\frac{1 - x^{2n} 1 + q^n}{1 + x^{2n} 1 - q^n} \right)^2 \quad [67]$$

This cannot be obtained by a direct application of CTMs but was conjectured by Baxter and Kelland and subsequently derived by Jimbo, Miwa, and Nakayashiki using difference equations.

One-Point Functions of the Hard-Hexagon Model

For hard hexagons, the working is more complicated because one must keep track of the sublattice of the central spin σ_0 , but fascinating connections emerge with the Rogers–Ramanujan functions:

$$\begin{aligned} G(x) &= \prod_{n=1}^{\infty} \frac{1}{(1 - x^{5n-4})(1 - x^{5n-1})} \\ H(x) &= \prod_{n=1}^{\infty} \frac{1}{(1 - x^{5n-3})(1 - x^{5n-2})} \end{aligned} \quad [68]$$

For hard hexagons, Baxter showed that

$$\rho_k = \frac{\text{tr } S(A_k B_k)^2}{\text{tr } (A_k B_k)^2} = \frac{\sum_{\sigma} \sigma_0 r_0^{2\sigma_0} w_0^{2E_{\sigma}}}{\sum_{\sigma} r_0^{2\sigma_0} w_0^{2E_{\sigma}}} \quad [69]$$

where $k=1,2,3$ labels the sublattice of the triangular lattice. Here the spin configurations $\sigma = (\sigma_0, \sigma_1, \sigma_3, \dots)$ with $\sigma_j = 0, 1$ are subject to the constraint $\sigma_j \sigma_{j+1} = 0$ for all j . If $|q^2| = e^{-\epsilon}$ and $g(x) = H(x)/G(x)$ then

$$\begin{aligned} x &= -e^{-\pi^2/5\epsilon}, \quad r_0^2 = -x/g(x), \quad w_0 = -x^3 \quad \text{for } z \leq z_c \\ x &= e^{-4\pi^2/5\epsilon}, \quad r_0^2 = x^{-1}g(x), \quad w_0 = x^{-3/2} \quad \text{for } z > z_c \end{aligned} \quad [70]$$

and

$$E_{\sigma} = \begin{cases} \sum_{j=1}^{\infty} j(\sigma_j - s_j), & z \leq z_c \\ \sum_{j=1}^{\infty} j(\sigma_j - \sigma_{j-1}\sigma_{j+1} - s_j + s_{j-1}s_{j+1}), & z > z_c \end{cases} \quad [71]$$

For large N , $\sigma_j \rightarrow s_j$, where the ground-state values s_j determined by the boundary conditions are

$$z \leq z_c: \quad s_j = 0 \quad [72]$$

$$z > z_c: \quad s_{3j+k} = 1, \quad s_{3j+k\pm 1} = 0, \quad k = 1, 2, 3 \quad [73]$$

After applying some Rogers–Ramanujan identities and introducing the elliptic functions

$$\begin{aligned} Q(x) &= \prod_{n=1}^{\infty} (1 - x^n) \\ P(x) &= \frac{Q(x)}{Q(x^2)} = \prod_{n=1}^{\infty} (1 - x^{2n-1}) \end{aligned} \quad [74]$$

the expressions for the sublattice densities simplify in the limit of large N giving

$$\rho = \rho_1 = \rho_2 = \rho_3 = -\frac{xG(x)H(x^6)P(x^3)}{P(x^2)}, \quad z \leq z_c \quad [75]$$

in the disordered fluid phase and

$$\begin{aligned} \rho_1 &= \frac{H(x)Q(x)[G(x)Q(x) + x^2H(x^9)Q(x^9)]}{Q(x^3)^2} \\ \rho_2 = \rho_3 &= \frac{x^2H(x)H(x^9)Q(x)Q(x^9)}{Q(x^3)^2} \end{aligned} \quad [76]$$

$$\begin{aligned} R = \rho_1 - \rho_2 &= \frac{Q(x)Q(x^5)}{Q(x^3)^2} \\ &= \prod_{n=1}^{\infty} \frac{(1 - x^n)(1 - x^{5n})}{(1 - x^{3n})^2}, \quad z > z_c \end{aligned} \quad [77]$$

in the triangular ordered phase. In principle, the dependence on x can be eliminated by observing that

$$z = \begin{cases} -x[H(x)/G(x)]^5, & z \leq z_c \\ x^{-1}[G(x)/H(x)]^5, & z > z_c \end{cases} \quad [78]$$

In practice, this is quite nontrivial. Although it is far from obvious, because $x \rightarrow 1$ is a subtle limit, the critical exponent associated with the order parameter R is

$$R \sim (z - z_c)^\beta \sim (q^2)^\beta, \quad \beta = 1/9 \quad [79]$$

Summary

Baxter's exact solutions of the eight-vertex and hard-hexagon models have been reviewed. These prototypical examples clearly illustrate the mathematical power and elegance of commuting transfer matrices and Yang–Baxter techniques. The results for the principal thermodynamic quantities, including free energies, correlation lengths, interfacial tensions, and one-point functions, have been summarized. For convenience in comparison, the associated critical exponents are collected in Table 1. All these exponents confirm the hyperscaling relation $2 - \alpha = d\nu$ for lattice dimensionality $d = 2$.

More recently, Yang–Baxter techniques have been applied to solve an infinite variety of lattice models in two dimensions. Commuting transfer methods have

Table 1 Comparison of the exactly calculated critical exponents of the rectangular Ising, eight-vertex and hard-hexagon models. The rectangular Ising model corresponds to the special case $\bar{\mu} = \pi/2$ of the eight-vertex model. The eight-vertex exponents vary continuously with $0 < \bar{\mu} < \pi$. The critical exponents of the hard-hexagon model, with its S_3 symmetry, lie in the universality class of the three-state Potts model.

Model	α	β	ν	μ
Rectangular Ising	0_{\log}	1/8	1	1
Eight vertex	$2 - \pi/\bar{\mu}$	$\pi/16\bar{\mu}$	$\pi/2\bar{\mu}$	$\pi/2\bar{\mu}$
Hard hexagons	1/3	1/9	5/6	5/6

also been adapted to study integrable boundaries and associated boundary critical behavior. Lastly, it should be mentioned that, in the continuum scaling limit, there are deep connections with conformal field theory and integrable quantum field theory. On the one hand, the lattice can often provide a convenient way to regularize the infinities that occur in these continuous field theories. On the other hand, the field theories can predict and explain the universal properties of lattice models such as critical exponents.

See also: Bethe Ansatz; Boundary Conformal Field Theory; Hopf Algebras and q -Deformation Quantum Groups; Integrability and Quantum Field Theory; q -Special Functions; Quantum Spin Systems; Two-Dimensional Ising Model; Yang–Baxter Equations.

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Einstein Equations: Exact Solutions

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Introduction

Even in a linear theory like Maxwell's electrodynamics, in which sufficiently general solutions of the field equations can be obtained, one needs a good sample, a useful kit, of explicit exact fields like the homogeneous field, the Coulomb monopole field, the dipole, and other simple solutions, in order to gain a physical intuition and understanding of the theory. In Einstein's general relativity, with its nonlinear field equations, the discoveries and analyses of various specific explicit solutions revealed most of the unforeseen features of the theory. Studies of special solutions stimulated questions relevant to more general situations, and even after the formulation of a conjecture about a general situation, newly discovered solutions can play a significant role in verifying or modifying the conjecture. The cosmic censorship conjecture assuming that "singularities forming in a realistic gravitational collapse are hidden inside horizons" is a good illustration.

Albert Einstein presented the final version of his gravitational field equations (or the Einstein's equations, EEs) to the Prussian Academy in Berlin on 18 November 1915:

$$R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R = \frac{8\pi G}{c^4}T_{\mu\nu} \quad [1]$$

Here, the spacetime metric tensor $g_{\mu\nu}(x^\rho)$, $\mu, \nu, \rho, \dots = 0, 1, 2, 3$, determines the invariant line element $g = g_{\mu\nu}dx^\mu dx^\nu$, and acts also as a dynamical variable describing the gravitational field; the Ricci tensor $R_{\mu\nu} = g^{\rho\sigma}R_{\rho\mu\sigma\nu}$, where $g^{\mu\rho}g_{\rho\nu} = \delta^\mu_\nu$, is formed from the Riemann curvature tensor $R_{\rho\mu\sigma\nu}$; both depend nonlinearly on $g_{\alpha\beta}$ and $\partial_\mu g_{\alpha\beta}$, and linearly on $\partial_\mu \partial_\nu g_{\alpha\beta}$; the scalar curvature $R = g^{\mu\nu}R_{\mu\nu}$. $T_{\mu\nu}(x^\rho)$ is the energy-momentum tensor of matter ("sources"); and Newton's gravitational constant G and the velocity of light c are fundamental constants. If not stated otherwise, we use the geometrized units in which $G = c = 1$, and the same conventions as in Misner *et al.* (1973) and Wald (1984). For example, in the case of perfect fluid with density ρ , pressure p , and 4-velocity U^μ , the energy-momentum tensor reads $T_{\mu\nu} = (\rho + p)U_\mu U_\nu + pg_{\mu\nu}$. To obtain a (local) solution of [1] in coordinate patch $\{x^\rho\}$ means to find "physically plausible" (i.e., complying with one of the positive-energy conditions) functions

$\rho(x^\rho), p(x^\rho), U_\mu(x^\rho)$, and metric $g_{\mu\nu}(x^\rho)$ satisfying [1]. In vacuum $T_{\mu\nu} = 0$ and [1] implies $R_{\mu\nu} = 0$.

In 1917, Einstein generalized [1] by adding a cosmological term $\Lambda g_{\mu\nu}$ ($\Lambda = \text{const.}$):

$$R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R + \Lambda g_{\mu\nu} = 8\pi T_{\mu\nu} \quad [2]$$

A homogeneous and isotropic static solution of [2] (with metric [8], $k = +1, a = \text{const.}$), in which the "repulsive effect" of $\Lambda > 0$ compensates the gravitational attraction of incoherent dust ("uniformly distributed galaxies") – the Einstein static universe – marked the birth of modern cosmology. Although it is unstable and lost its observational relevance after the discovery of the expansion of the universe in the late 1920s, in 2004 a "fine-tuned" cosmological scenario was suggested according to which our universe starts asymptotically from an initial Einstein static state and later enters an inflationary era, followed by a standard expansion epoch (see Cosmology: Mathematical Aspects). There are many other examples of "old" solutions which turned out to act as asymptotic states of more general classes of models.

Invariant Characterization and Classification of the Solutions

Algebraic Classification

The Riemann tensor can be decomposed as

$$R_{\alpha\beta\gamma\delta} = C_{\alpha\beta\gamma\delta} + E_{\alpha\beta\gamma\delta} + G_{\alpha\beta\gamma\delta} \quad [3]$$

where E and G are constructed from $R_{\alpha\beta}$, R , and $g_{\alpha\beta}$ (see, e.g., Stephani *et al.* (2003)); the Weyl conformal tensor $C_{\alpha\beta\gamma\delta}$ can be considered as the "characteristic of the pure gravitational field" since, at a given point, it cannot be determined in terms of the matter energy-momentum tensor $T_{\alpha\beta}$ (as E and G can using EEs). Algebraic classification is based on a classification of the Weyl tensor. This is best formulated using two-component spinors α_A ($A = 1, 2$), in terms of which any Weyl spinor Ψ_{ABCD} determining $C_{\alpha\beta\gamma\delta}$ can be factorized:

$$\Psi_{ABCD} = \alpha_{(A}\beta_B\gamma_C\delta_{D)} \quad [4]$$

brackets denote symmetrization; each of the spinors determines a principal null direction, say, $k^\alpha = \alpha^A \bar{\alpha}^{A'}$ (see Spinors and Spin Coefficients). The Petrov–Penrose classification is based on coincidences among these directions. A solution is of type *I* (general case), *II*, *III*, and *N* ("null") if all null directions are different, or two, three, and all four coincide, respectively. It is of type *D* ("degenerate")

if there are two double null directions. The equivalent tensor equations are simplest for type N:

$$\begin{aligned} C_{\alpha\beta\gamma\delta}k^\delta &= 0, & C_{\alpha\beta\gamma\delta}C^{\alpha\beta\gamma\delta} &= 0, \\ C_{\alpha\beta\gamma\delta}C^{*\alpha\beta\gamma\delta} &= 0 \end{aligned} \quad [5]$$

where $C_{\alpha\beta\gamma\delta}^* = (1/2)\epsilon_{\alpha\beta\rho\sigma}C^{\rho\sigma}_{\gamma\delta}$, ϵ is the Levi-Civita pseudotensor.

Classification According to Symmetries

Most of the available solutions have some exact continuous symmetries which preserve the metric. The corresponding group of motions is characterized by the number and properties of its Killing vectors ξ^α satisfying the Killing equation $(\mathcal{L}_\xi g)_{\alpha\beta} = \xi_{\alpha;\beta} + \xi_{\beta;\alpha} = 0$ (\mathcal{L} is the Lie derivative) and by the nature (spacelike, timelike, or null) of the group orbits. For example, axisymmetric, stationary fields possess two commuting Killing vectors, of which one is timelike. Orbits of the axial Killing vector are closed spacelike curves of finite length, which vanishes at the axis of symmetry. In cylindrical symmetry, there exist two spacelike commuting Killing vectors. In both cases, the vectors generate a two-dimensional abelian group. The two-dimensional group orbits are timelike in the stationary case and spacelike in the cylindrical symmetry.

If a timelike ξ^α is hypersurface orthogonal, $\xi_\alpha = \lambda\Phi_{,\alpha}$ for some scalar functions λ, Φ , the spacetime is “static.” In coordinates with $\xi = \partial_t$, the metric is

$$g = -e^{2U}dt^2 + e^{-2U}\gamma_{ik}dx^i dx^k \quad [6]$$

where U, γ_{ik} do not depend on t . In vacuum, U satisfies the potential equation $U_{;a}^{:a} = 0$, the covariant derivatives (denoted by $:$) are with respect to the three-dimensional metric γ_{ik} . A classical result of Lichnerowicz states that if the vacuum metric is smooth everywhere and $U \rightarrow 0$ at infinity, the spacetime is flat (for refinements, see Anderson (2000)).

In cosmology, we are interested in groups whose regions of transitivity (points can be carried into one another by symmetry operations) are three-dimensional spacelike hypersurfaces (homogeneous but anisotropic models of the universe). The three-dimensional simply transitive groups G_3 were classified by Bianchi in 1897 according to the possible distinct sets of structure constants but their importance in cosmology was discovered only in the 1950s. There are nine types: Bianchi I to Bianchi IX models. The line element of the Bianchi universes can be expressed in the form

$$g = -dt^2 + g_{ab}(t)\omega^a\omega^b \quad [7]$$

where the time-independent 1-forms $\omega^a = E_\alpha^a dx^\alpha$ satisfy the relations $d\omega^a = -(1/2)C_{bc}^a\omega^b \wedge \omega^c$, d is

the exterior derivative and C_{bc}^a are the structure constants (see Cosmology: Mathematical Aspects for more details).

The standard Friedmann–Lemaître–Robertson–Walker (FLRW) models admit in addition an isotropy group $SO(3)$ at each point. They can be represented by the metric

$$g = -dt^2 + [a(t)]^2 \left(\frac{dr^2}{1-kr^2} + r^2(d\theta^2 + \sin^2\theta d\varphi^2) \right) \quad [8]$$

in which $a(t)$, the “expansion factor,” is determined by matter via EEs, the curvature index $k = -1, 0, +1$, the three-dimensional spaces $t = \text{const.}$ have a constant curvature $K = k/a^2$; $r \in [0, 1]$ for closed ($k = +1$) universe, $r \in [0, \infty)$ in open ($k = 0, -1$) universes (for another description (see Cosmology: Mathematical Aspects)).

There are four-dimensional spacetimes of constant curvature solving EEs [2] with $T_{\mu\nu} = 0$: the Minkowski, de Sitter, and anti-de Sitter spacetimes. They admit the same number [10] of independent Killing vectors, but interpretations of the corresponding symmetries differ for each spacetime.

If ξ^α satisfies $\mathcal{L}_\xi g_{\alpha\beta} = 2\Phi g_{\alpha\beta}$, $\Phi = \text{const.}$, it is called a homothetic (Killing) vector. Solutions with proper homothetic motions, $\Phi \neq 0$, are “self-similar.” They cannot in general be asymptotically flat or spatially compact but can represent asymptotic states of more general solutions. In Stephani *et al.* (2003), a summary of solutions with proper homotheties is given; their role in cosmology is analyzed by Wainwright and Ellis (eds.) (1997); for mathematical aspects of symmetries in general relativity, see Hall (2004).

There are other schemes for invariant classification of exact solutions (reviewed in Stephani *et al.* (2003)): the algebraic classification of the Ricci tensor and energy–momentum tensor of matter; the existence and properties of preferred vector fields and corresponding congruences; local isometric embeddings into flat pseudo-Euclidean spaces, etc.

Minkowski (M), de Sitter (dS), and Anti-de Sitter (AdS) Spacetimes

These metrics of constant (zero, positive, negative) curvature are the simplest solutions of [2] with $T_{\mu\nu} = 0$ and $\Lambda = 0, \Lambda > 0, \Lambda < 0$, respectively. The standard topology of M is R^4 . The dS has the topology $R^1 \times S^3$ and is best represented as a four-dimensional hyperboloid $-v^2 + w^2 + x^2 + y^2 + z^2 = (3/\Lambda)$ in a five-dimensional flat space with metric $g = -dv^2 + dw^2 + dx^2 + dy^2 + dz^2$. The AdS has the topology $S^1 \times R^3$; it is a four-dimensional hyperboloid $-v^2 - w^2 + x^2 + y^2 + z^2 = -(3/\Lambda), \Lambda < 0$, in flat five-dimensional space

with signature $(-, -, +, +, +)$. By unwrapping the circle S^1 and considering the universal covering space, one gets rid of closed timelike lines.

These spacetimes are all conformally flat and can be conformally mapped into portions of the Einstein universe (see Asymptotic Structure and Conformal Infinity). However, their conformal structure is globally different. In M , one can go to infinity along timelike/null/spacelike geodesics and reach five qualitatively different sets of points: future/past timelike infinity i^\pm , future/past null infinity \mathcal{I}^\pm , and spacelike infinity i^0 . In dS , there are only past and future conformal infinities $\mathcal{I}^-, \mathcal{I}^+$, both being spacelike (on the Einstein cylinder, the dS spacetime is a “horizontal strip” with $\mathcal{I}^+/\mathcal{I}^-$ as the “upper/lower circle”). The conformal infinity in AdS is timelike.

As a consequence of spacelike \mathcal{I}^\pm in dS , there exist both particle (cosmological) and event horizons for geodesic observers (Hawking and Ellis 1973). dS plays a (doubly) fundamental role in the present-day cosmology: it is an approximate model for inflationary paradigm near the big bang and it is also the asymptotic state (at $t \rightarrow \infty$) of cosmological models with a positive cosmological constant. Since recent observations indicate that $\Lambda > 0$, it appears to describe the future state of our universe. AdS has come recently to the fore due to the “holographic” conjecture (see AdS/CFT Correspondence).

Christodoulou and Klainermann, and Friedrich proved that M , dS , and AdS are stable with respect to general, nonlinear (though “weak”) vacuum perturbations – result not known for any other solution of EEs (see Stability of Minkowski Space).

Schwarzschild and Reissner–Nordström Metrics

These are spherically symmetric spacetimes – the SO_3 rotation group acts on them as an isometry group with spacelike, two-dimensional orbits. The metric can be brought into the form

$$g = -e^{2\nu} dt^2 + e^{2\lambda} dr^2 + r^2(d\theta^2 + \sin^2\theta d\varphi^2) \quad [9]$$

$\nu(t, r), \lambda(t, r)$ must be determined from EEs. In vacuum, we are led uniquely to the Schwarzschild metric

$$g = -\left(1 - \frac{2M}{r}\right) dt^2 + \left(1 - \frac{2M}{r}\right)^{-1} dr^2 + r^2(d\theta^2 + \sin^2\theta d\varphi^2) \quad [10]$$

where $M = \text{const.}$ has to be interpreted as mass, as test particle orbits show. The spacetime is static at $r > 2M$, that is, outside the Schwarzschild radius at $r = 2M$, and asymptotically ($r \rightarrow \infty$) flat.

Metric [10] describes the exterior gravitational field of an arbitrary (static, oscillating, collapsing, or expanding) spherically symmetric body (spherically symmetric gravitational waves do not exist). It is the most influential solution of EEs. The essential tests of general relativity – perihelion advance of Mercury, deflection of both optical and radio waves by the Sun, and signal retardation – are based on [10] or rather on its expansion in M/r . Space missions have been proposed that could lead to measurements of “post-post-Newtonian” effects (see General Relativity: Experimental Tests, and Misner *et al.* (1973)). The full Schwarzschild metric is of importance in astrophysical processes involving compact stars and black holes.

Metric [10] describes the spacetime outside a spherical body collapsing through $r = 2M$ into a spherical black hole. In Figure 1, the formation of an event horizon and trapped surfaces is indicated in ingoing Eddington–Finkelstein coordinates (v, r, θ, φ) where $v = t + r + 2M \log(r/2M - 1)$ so that $(v, \theta, \varphi) = \text{const.}$ are ingoing radial null geodesics. The interior of the star is described by another metric (e.g., the Oppenheimer–Snyder collapsing dust solution – see below). The Kruskal extension of the Schwarzschild solution, its compactification, the concept of the bifurcate Killing horizon, etc., are analyzed

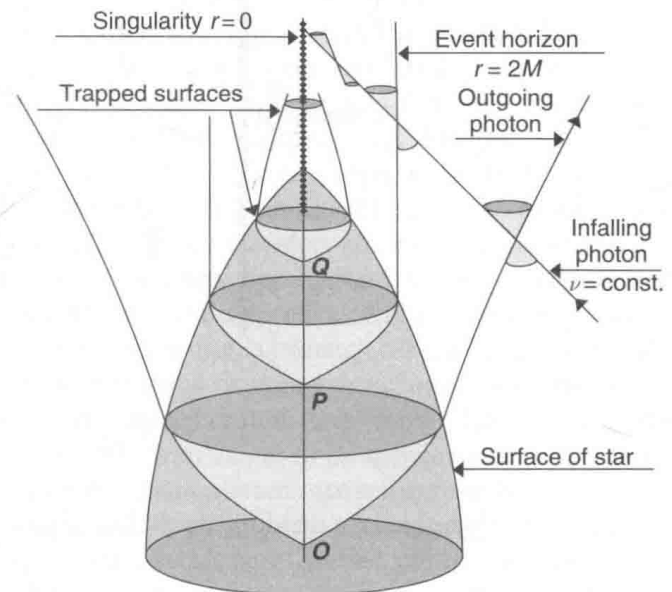


Figure 1 Gravitational collapse of a spherical star (the interior of the star is shaded). The light cones of three events, O , P , Q , at the center of the star, and of three events outside the star are illustrated. The event horizon, the trapped surfaces, and the singularity formed during the collapse are also shown. Although the singularity appears to lie along the direction of time, from the character of the light cone outside the star but inside the event horizon we can see that it has a spacelike character. Reproduced from Bičák J (2000) Selected solutions of Einstein's field equations: their role in general relativity and astrophysics. In: Schmidt BG (ed.) *Einstein's Field Equations and their physical Implications*. Lecture Notes in Physics, vol. 540, pp. 1–126. Heidelberg: Springer, with permission from Springer-Verlag.

in Stationary Black Holes and in Misner *et al.* (1973), Hawking and Ellis (1973), and Bičák (2000).

The Reissner–Nordström solution describes the exterior gravitational and electromagnetic fields of a spherical body with mass M and charge Q . The energy-momentum tensor on the right-hand side of EE [2] is that of the electromagnetic field produced by the charge; the field satisfies the curved-space Maxwell equations. The metric reads

$$g = -\left(1 - \frac{2M}{r} + \frac{Q^2}{r^2}\right) dt^2 + \left(1 - \frac{2M}{r} + \frac{Q^2}{r^2}\right)^{-1} dr^2 + r^2(d\theta^2 + \sin^2\theta d\varphi^2) \quad [11]$$

The analytic extension of the electrovacuum metric [11] is qualitatively different from the Kruskal extension of the Schwarzschild metric. In the case $Q^2 > M^2$ there is a “naked singularity” (visible from $r \rightarrow \infty$) at $r=0$ where curvature invariants diverge. If $Q^2 < M^2$, the metric describes a (generic) static charged black

hole with two event horizons at $r=r_{\pm} = M \pm (M^2 - Q^2)^{1/2}$. The Killing vector $\partial/\partial t$ is null at the horizons, timelike at $r > r_+$ and $r < r_-$, but spacelike between the horizons. The character of the extended spacetime is best seen in the compactified form, Figure 2, in which world-lines of radial light rays are 45° lines. Again, two infinities (right and left, in regions I and III) arise (as in the Kruskal–Schwarzschild diagram, see Stationary Black Holes), however, the maximally extended geometry consists of an infinite chain of asymptotically flat regions connected by “wormholes” between the singularities at $r=0$. In contrast to the Schwarzschild singularity, the singularities are timelike – they do not block the way to the future. The inner horizon $r=r_-$ represents a Cauchy horizon for a typical initial hypersurface like Σ (Figure 2): what is happening in regions V is in general influenced not only by data on Σ but also at the singularities. The Cauchy horizon is unstable (for references, see Bičák (2000) and recent work by Dafermos (2005)).

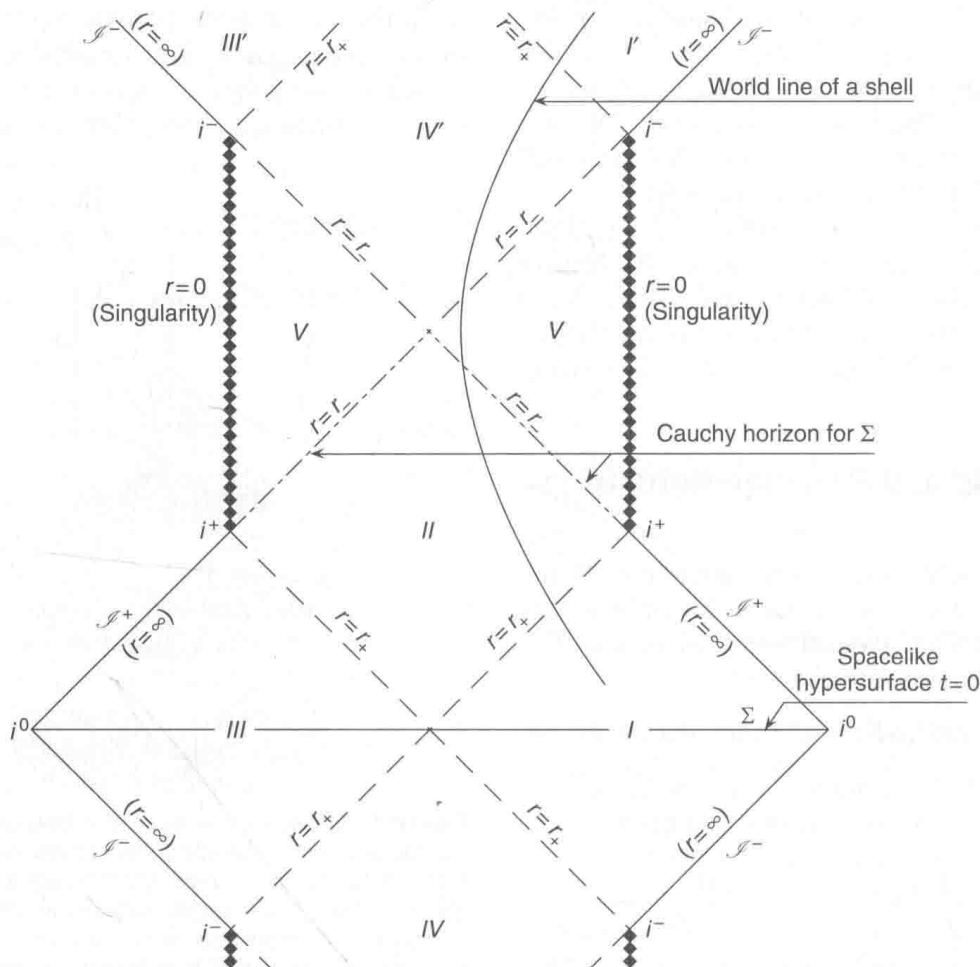


Figure 2 The compactified Reissner–Nordström spacetime representing a non-extreme black hole consists of an infinite chain of asymptotic regions (“universes”) connected by “wormholes” between timelike singularities. The world-line of a shell collapsing from “universe” I and re-emerging in “universe” I’ is indicated. The inner horizon at $r=r_-$ is the Cauchy horizon for a spacelike hypersurface Σ . It is unstable and thus it will very likely prevent such a process. Reproduced from Bičák J (2000) Selected solutions of Einstein’s field equations: their role in general relativity and astrophysics. In: Schmidt BG (ed.) *Einstein’s Field Equations and their Physical Implications*, Lecture Notes in Physics, vol. 540, pp. 1–126. Heidelberg: Springer, with permission from Springer-Verlag.

For $M^2 = Q^2$ the two horizons coincide at $r_+ = r_- = M$. Metric [11] describes extreme Reissner–Nordström black holes. The horizon becomes degenerate and its surface gravity vanishes (see Stationary Black Holes). Extreme black holes play a significant role in string theory (Ortín 2004).

Stationary Axisymmetric Solutions

Assume the existence of two commuting Killing vectors – timelike ξ^α and axial η^α ($\xi^\alpha \xi_\alpha < 0, \eta^\alpha \eta_\alpha > 0$), ξ^α normalized at (asymptotically flat) infinity, η^α at the rotation axis. They generate two-dimensional orbits of the group G_2 . Assume there exist 2-spaces orthogonal to these orbits. This is true in vacuum and also in case of electromagnetic fields or perfect fluids whose 4-current or 4-velocity lies in the surfaces of transitivity of G_2 (e.g., toroidal magnetic fields are excluded). The metric can then be written in Weyl’s coordinates (t, ρ, φ, z)

$$g = -e^{2U}(dt + A d\varphi)^2 + e^{-2U}[e^{2k}(d\rho^2 + dz^2) + \rho^2 d\varphi^2] \quad [12]$$

U, k , and A are functions of ρ, z .

The most celebrated vacuum solution of the form [12] is the Kerr metric for which U, k, A are ratios of simple polynomials in spheroidal coordinates (simply related to (ρ, z)). The Kerr solution is characterized by mass M and specific angular momentum a . For $a^2 > M^2$, it describes an asymptotically flat spacetime with a naked singularity. For $a^2 \leq M^2$, it represents a rotating black hole that has two horizons which coalesce into a degenerate horizon for $a^2 = M^2$ – an extreme Kerr black hole. The two horizons are located at $r_\pm = M \pm (M^2 - a^2)^{1/2}$ (r being the Boyer–Lindquist coordinate (see Stationary Black Holes)). As with the Reissner–Nordström black hole, the singularity inside is timelike and the inner horizon is an (unstable) Cauchy horizon. The analytic extension of the Kerr metric resembles Figure 2 (see Frolov and Novikov (1998), Hawking and Ellis (1973), Misner *et al.* (1973), Ortín (2004), Semerák *et al.* (2002), Stephani *et al.* (2003), and Wald (1984) for details).

Thanks to the black hole uniqueness theorems (see Stationary Black Holes), the Kerr metric is the unique solution describing all rotating black holes in vacuum. If the cosmic censorship conjecture holds, Kerr black holes represent the end states of gravitational collapse of astronomical objects with supercritical masses. According to prevalent views, they reside in the nuclei of most galaxies. Unlike with a spherical collapse, there are no exact solutions available which would represent the formation of a Kerr black hole. However,

starting from metric [12] and identifying, for example, $z = b = \text{const.}$ and $z = -b$ (with the region $-b < z < b$ being cut off), one can construct thin material disks which are physically plausible and can be the sources of the Kerr metric even for $a^2 > M^2$ (see Bičák (2000) for details).

In a general case of metric [12], EEs in vacuum imply the “Ernst equation” for a complex function f of ρ and z :

$$(\Re f) \left[f_{,\rho\rho} + f_{,zz} + \frac{1}{\rho} f_{,\rho} \right] = f_{,\rho}^2 + f_{,z}^2 \quad [13]$$

or, equivalently, $(\Re f) \Delta f = (\nabla f)^2$, where $f = e^{2U} + ib$, U enters [12], and $b(\rho, z)$ is a “potential” for $A(\rho, z)$: $A_{,\rho} = \rho e^{-4U} b_{,z}$, $A_{,z} = -\rho e^{-4U} b_{,\rho}$; $k(\rho, z)$ in [12] can be determined from U and b by quadratures. Tomimatsu and Sato (TS) exploited symmetries of [13] to construct metrics generalizing the Kerr metric. Replacing f by $\xi = (1 - f)/(1 + f)$, one finds that in case of the Kerr metric ξ^{-1} is a linear function in the prolate spheroidal coordinates, whereas for TS solutions ξ is a quotient of higher-order polynomials. A number of other solutions of eqn [13] were found but they are of lower significance than the Kerr solution (cf. Stephani *et al.* (2003), Chapter 20).

These solutions inspired “solution-generating methods” in general relativity. The Ernst equation can be regarded as the integrability condition of a system of linear differential equations. The problem of solving such a system can be reformulated as the Riemann–Hilbert problem in complex function theory (see Riemann–Hilbert Problem and Integrable Systems: Overview). We refer to Stephani *et al.* (2003) and Belinski and Verdaguer (2001) where these techniques using Bäcklund transformations, inverse-scattering method, etc., are also applied in the nonstationary context of two spacelike Killing vectors (waves, cosmology). In the stationary case, all asymptotically flat, stationary, axisymmetric vacuum solutions can, in principle, be generated. It is known how to generate fields with given values of multipole moments, though the required calculations are staggering. By solving the Riemann–Hilbert problem with appropriate boundary data, Neugebauer and Meinel constructed the exact solution representing a rigidly rotating thin disk of dust (cf. Stephani *et al.* (2003) and Bičák (2000)).

A subclass of metrics [12] is formed by static Weyl solutions with $A = b = 0$. Equation [13] then becomes the Laplace equation $\Delta U = 0$. The non-linearity of EEs enters only the equations for k : $k_{,\rho} = \rho(U_{,\rho}^2 - U_{,z}^2)$, $k_{,z} = 2\rho U_{,\rho} U_{,z}$. The class contains some explicit solutions of interest: the “linear superposition” of collinear particles with string-like singularities between them which keep the system in static equilibrium; solutions representing external

fields of counter-rotating disks, for example, those which are “inspired” by galactic Newtonian potentials; disks around black holes and some other special solutions (Stephani *et al.* 2003, Bonnor 1992, Bičák 2000, Semerák *et al.* 2002).

There are solutions of the Einstein–Maxwell equations representing external fields of masses endowed with electric charges, magnetic dipole moments, etc. (Stephani *et al.* 2003). Best known is the Kerr–Newman metric characterized by parameters M , a , and charge Q . For $M^2 \geq a^2 + Q^2$ it describes a charged, rotating black hole. Owing to the rotation, the charged black hole produces also a magnetic field of a dipole type. All the black hole solutions can be generalized to include a nonvanishing Λ (for various applications, see Semerák *et al.* 2002)). Other generalizations incorporate the so-called Newman–Unti–Tamburino (NUT) parameter (corresponding to a “gravomagnetic monopole”) or an “external” magnetic/electric field or a parameter leading to “uniform” acceleration (see Stephani *et al.* (2003) and Bičák (2000)). Much interest has recently been paid to black hole (and other) solutions with various types of gauge fields and to multidimensional solutions. References Frolov and Novikov (1998) and Ortín (2004) are two examples of good reviews.

Radiative Solutions

Plane Waves and Their Collisions

The best-known class are “plane-fronted gravitational waves with parallel rays” (pp-waves) which are defined by the condition that the spacetime admits a covariantly constant null vector field $k^\alpha: k_{\alpha;\beta} = 0$. In suitable null coordinates u, v such that $k_\alpha = u_{,\alpha}$, $k^\alpha = (\partial/\partial v)^\alpha$, and complex coordinate ζ which spans the wave 2-surfaces $u = \text{const.}$, $v = \text{const.}$ with Euclidean geometry, the metric reads

$$g = 2d\zeta d\bar{\zeta} - 2dudv - 2H(u, \zeta, \bar{\zeta})du^2 \quad [14]$$

$H(u, \zeta, \bar{\zeta})$ is a real function. The vacuum EEs imply $H_{,\zeta\bar{\zeta}} = 0$ so that $2H = f(u, \zeta) + \bar{f}(u, \bar{\zeta})$, f is an arbitrary function of u , analytic in ζ . The Weyl tensor satisfies eqns [5] – the field is of type N as is the field of plane electromagnetic waves. In the null tetrad $\{k^\alpha, l^\alpha, m^\alpha(\text{complex})\}$ with $l^\alpha k_\alpha = -1$, $m^\alpha \bar{m}_\alpha = 1$, all other products vanishing, the only nonzero projection of the Weyl tensor, $\Psi = C_{\alpha\beta\gamma\delta} l^\alpha \bar{m}^\beta l^\gamma m^\delta = H_{,\zeta\bar{\zeta}}$, describes the transverse component of a wave propagating in the k^α direction. Writing $\Psi = A e^{i\Theta}$, the real $A > 0$ is the amplitude of the wave, Θ describes polarization. Waves with $\Theta = \text{const.}$ are called linearly polarized. Considering their effect on test particles, one finds that plane waves are transverse.

The simplest waves are homogeneous in the sense that Ψ is constant along the wave surfaces. One gets $f(u, \zeta) = (1/2)A(u)e^{i\Theta(u)}\zeta^2$. Instructive are “sandwich waves,” for example, waves with a “square profile”: $A = 0$ for $u < 0$ and $u > a^2$, $A = a^{-2} = \text{const.}$ for $0 \leq u \leq a^2$. This example demonstrates, within exact theory, that the waves travel with the speed of light, produce relative accelerations of test particles, focus astigmatically generally propagating parallel rays, etc. The focusing effects have a remarkable consequence: there exists no global spacelike hypersurface on which initial data could be specified – plane wave spacetimes contain no global Cauchy hypersurface.

“Impulsive” plane waves can be generated by boosting a “particle” at rest to the velocity of light by an appropriate limiting procedure. The ultrarelativistic limit of, for example, the Schwarzschild metric (the so-called Aichelburg–Sexl solution) can be employed as a “limiting incoming state” in black hole encounters (cf. monograph by d’Eath (1996)). Plane-fronted waves have been used in quantum field theory. For a review of exact impulsive waves, see Semerák *et al.* (2002).

A collision of plane waves represents an exceptional situation of nonlinear wave interactions which can be analyzed exactly. Figure 3 illustrates a typical case in which the collision produces a spacelike singularity. The initial-value problem with data given at $v = 0$ and $u = 0$ can be formulated in terms of the equivalent matrix Riemann–Hilbert problem (see Riemann–Hilbert Problem); it is related to the hyperbolic counterpart of the Ernst equation [13]. For reviews, see Griffiths (1991), Stephani *et al.* (2003), and Bičák (2000).

Cylindrical Waves

Discovered by G Beck in 1925 and known today as the Einstein–Rosen waves (1937), these vacuum solutions helped to clarify a number of issues, such as energy loss due to the waves, asymptotic structure of radiative

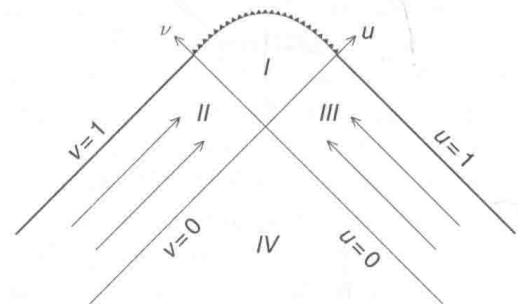


Figure 3 A spacetime diagram indicating a collision of two plane-fronted gravitational waves which come from regions II and III, collide in region I, and produce a spacelike singularity. Region IV is flat. Reproduced from Bičák J (2000) Selected solutions of Einstein's field equations: their role in general relativity and astrophysics. In: Schmidt BG (ed.) *Einstein's Field Equations and their Physical Implications*, Lecture Notes in Physics, vol. 540, pp. 1–126. Heidelberg: Springer, with permission from Springer-Verlag.

spacetimes, dispersion of waves, quasilocal mass-energy, cosmic censorship conjecture, or quantum gravity in the context of midisuperspaces (see Bičák (2000) and Belinski and Verdaguer (2001)).

In the metric

$$g = e^{2(\gamma-\psi)}(-dt^2 + d\rho^2) + e^{2\psi}dz^2 + \rho^2 e^{-2\psi}d\varphi^2 \quad [15]$$

$\psi(t, \rho)$ satisfies the flat-space wave equation and $\gamma(\rho, t)$ is given in terms of ψ by quadratures. Admitting a “cross term” $\sim \omega(t, \rho) dz d\phi$, one acquires a second degree of freedom (a second polarization) which makes all field equations nonlinear.

Boost-Rotation Symmetric Spacetimes

These are the only explicit solutions available which are radiative and represent the fields of finite sources. Figure 4 shows two particles uniformly accelerated in opposite directions. In the space diagram (left), the “string” connecting the particles is the “cause” of the acceleration. In “Cartesian-type” coordinates and the z -axis chosen as the symmetry axis, the boost Killing vector has a flat-space form, $\zeta = z(\partial/\partial t) + t(\partial/\partial z)$, the same is true for the axial Killing vector. The metric contains two functions of variables $\rho^2 \equiv x^2 + y^2$ and $\beta^2 \equiv z^2 - t^2$. One satisfies the flat-space wave equation, the other is determined by quadratures.

The unique role of these solutions is exhibited by the theorem which states that in axially symmetric, locally asymptotically flat spacetimes, in the sense that a null infinity (see Asymptotic Structure and Conformal Infinity) exists but not necessarily globally, the only additional symmetry that does not exclude gravitational

radiation is the boost symmetry. Various radiation characteristics can be expressed explicitly in these spacetimes. They have been used as tests in numerical relativity and approximation methods. The best-known example is the C-metric (representing accelerating black holes, in general charged and rotating, and admitting Λ), see Bonnor *et al.* (1994), Bičák (2000), Stephani *et al.* (2003), and Semerák *et al.* (2002).

Robinson–Trautman Solutions

These solutions are algebraically special but in general they do not possess any symmetry. They are governed by a function $P(u, \zeta, \bar{\zeta})$ (u is the retarded time, ζ a complex spatial coordinate) which satisfies a fourth-order nonlinear parabolic differential equation. Studies by Chruściel and others have shown that RT solutions of Petrov type II exist globally for all positive “times” u and converge asymptotically to a Schwarzschild metric, though the extension across the “Schwarzschild-like” horizon can only be made with a finite degree of smoothness. Generalization to the cases with $\Lambda > 0$ gives explicit models supporting the cosmic no-hair conjecture (an exponentially fast approach to the dS spacetime) under the presence of gravitational waves. See Bonnor *et al.* (1994), Bičák (2000), and Stephani *et al.* (2003).

Material Sources

Finding physically sound material sources in an analytic form even for some simple vacuum metrics remains an open problem. Nevertheless, there are solutions representing regions of spacetimes filled with matter which are of considerable interest.

One of the simplest solutions, the spherically symmetric Schwarzschild interior solution with incompressible fluid as its source, represents “a star” of uniform density, $\rho = \rho_0 = \text{const.}$:

$$g = - \left[\frac{3}{2} \sqrt{1 - AR^2} - \frac{1}{2} \sqrt{1 - Ar^2} \right]^2 dt^2 + \frac{dr^2}{1 - Ar^2} + r^2(d\theta^2 + \sin^2 \theta d\varphi^2) \quad [16]$$

$A = 8\pi\rho_0/3 = \text{const.}$, R is the radius of the star.

The equation of hydrostatic equilibrium yields pressure inside the star:

$$8\pi p = 2A \frac{\sqrt{1 - Ar^2} - \sqrt{1 - AR^2}}{3\sqrt{1 - AR^2} - \sqrt{1 - Ar^2}} \quad [17]$$

Solution [16] can be matched at $r = R$, where $p = 0$, to the exterior vacuum Schwarzschild solution [10] if the Schwarzschild mass $M = (1/2)AR^3$. Although “incompressible fluid” implies an infinite speed of sound, the above solution provides an instructive

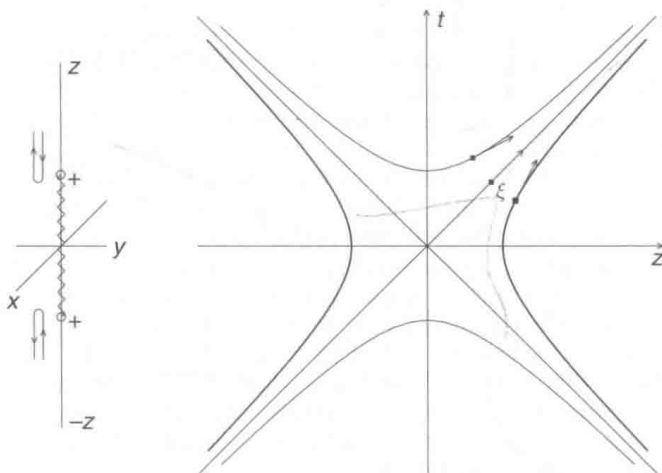


Figure 4 Two particles uniformly accelerated in opposite directions. Orbits of the boost Killing vector (thinner hyperbolas) are spacelike in the region $t^2 > z^2$. Reproduced from Bičák J (2000) Selected solutions of Einstein's field equations: their role in general relativity and astrophysics. In: Schmidt BG (ed.) *Einstein's Field Equations and their Physical Implications*, Lecture Notes in Physics, vol. 540, pp. 1–126. Heidelberg: Springer, with permission from Springer-Verlag.

model of relativistic hydrostatics. A Newtonian star of uniform density can have an arbitrarily large radius $R = \sqrt{3p_c/2\pi\rho_0^2}$ and mass $M = (p_c/\rho_0^2) \sqrt{6p_c/\pi}$, p_c is the central pressure. However, [17] implies that (1) M and R satisfy the inequality $2M/R \leq 8/9$, (2) equality is reached as p_c becomes infinite and R and M attain their limiting values $R_{\text{lim}} = (3\pi\rho_0)^{-1/2} = (9/4)M_{\text{lim}}$. For a density typical in neutron stars, $\rho_0 = 10^{15} \text{ g cm}^{-3}$, we get $M_{\text{lim}} \doteq 3.96M_\odot$ (M_\odot solar mass) – even this simple model shows that in Einstein’s theory neutron stars can only be a few solar masses. In addition, one can prove that the “Buchdahl’s inequality” $2M/R \leq 8/9$ is valid for an arbitrary equation of state $p = p(\rho)$. Only a limited mass can thus be contained within a given radius in general relativity. The gravitational redshift $z = (1 - 2M/R)^{-1/2} - 1$ from the surface of a static star cannot be higher than 2.

Many other explicit static perfect fluid solutions are known (we refer to Stephani *et al.* (2003) for a list), however, none of them can be considered as really “physical.” Recently, the dynamical systems approach to relativistic spherically symmetric static perfect fluid models was developed by Ugla and others which gives qualitative characteristics of masses and radii.

The most significant nonstatic spacetime describing a bounded region of matter and its external field is undoubtedly the Oppenheimer–Snyder model of “gravitational collapse of a spherical star” of uniform density and zero pressure (a “ball of dust”). The model does not represent any new (local) solution: the interior of the star is described by a part of a dust-filled FLRW universe (cf. [8]), the external region by the Schwarzschild vacuum metric (cf. eqn [10], Figure 1).

Since Vaidya’s discovery of a “radiating Schwarzschild metric,” null dust (“pure radiation field”) has been widely used as a simple matter source. Its energy–momentum tensor, $T_{\alpha\beta} = \rho k_\alpha k_\beta$, where $k_\alpha k^\alpha = 0$, may be interpreted as an incoherent superposition of waves with random phases and polarizations moving in a single direction, or as “lightlike particles” (photons, neutrinos, gravitons) that move along k^α . The “Vaidya metric” describing spherical implosion of null dust implies that in case of a “gentle” inflow of the dust, a naked singularity forms. This is relevant in the context of the cosmic censorship conjecture (cf., e.g., Joshi (1993)).

Cosmological Models

There exist important generalizations of the standard FLRW models other than the above-mentioned Bianchi models, particularly those that maintain spherical symmetry but do not require homogeneity. The best known are the Lemaître–Tolman–Bondi

models of inhomogeneous universes of pure dust, the density of which may vary (Kraśiński 1997).

Other explicit cosmological models of principal interest involve, for example, the Gödel universe – a homogeneous, stationary spacetime with $\Lambda < 0$ and incoherent rotating matter in which there exist closed timelike curves through every point; the Kantowski–Sachs solutions – possessing homogeneous spacelike hypersurfaces but (in contrast to the Bianchi models) admitting no simply transitive G_3 ; and vacuum Gowdy models (“generalized Einstein–Rosen waves”) admitting G_2 with compact 2-tori as its group orbits and representing cosmological models closed by gravitational waves. See Cosmology: Mathematical Aspects and references Stephani *et al.* (2003), Belinski and Verdaguer (2001), Bičák (2000), Hawking and Ellis (1973), Kraśiński (1997) and Wainwright and Ellis (1997).

See also: AdS/CFT Correspondence; Asymptotic Structure and Conformal Infinity; Cosmology: Mathematical Aspects; Dirac Fields in Gravitation and Nonabelian Gauge Theory; Einstein Manifolds; Einstein’s Equations with Matter; General Relativity: Experimental Tests; General Relativity: Overview; Hamiltonian Reduction of Einstein’s Equations; Integrable Systems: Overview; Newtonian Limit of General Relativity; Pseudo-Riemannian Nilpotent Lie Groups; Reimann–Hilbert Problem; Spacetime Topology, Causal Structure and Singularities; Spinors and Spin Coefficients; Stability of Minkowski Space; Stationary Black Holes; Twistor Theory: Some Applications.

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Einstein Equations: Initial Value Formulation

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Introduction

Einstein's theory of gravity models a gravitating physical system \mathcal{S} using a spacetime (M^4, g, ψ) which satisfies the Einstein field equations

$$G_{\mu\nu}(g) = \kappa T_{\mu\nu}(g, \psi) \quad [1]$$

$$\mathcal{F}(g, \psi) = 0 \quad [2]$$

Here, M^4 is a four-dimensional spacetime manifold, g is a Lorentz signature metric on M , ψ represents the nongravitational ("matter") fields of interest, $G_{\mu\nu} := R_{\mu\nu} - (1/2)g_{\mu\nu}R$ is the Einstein curvature tensor, κ is a constant, $T_{\mu\nu}$ is the stress-energy tensor for the field ψ , and $\mathcal{F} = 0$ represents the nongravitational field equations (e.g., $\nabla_\mu F^\mu_\nu = 0$ for the Einstein-Maxwell theory).

By far the most widely used way to obtain and to study spacetime solutions (M^4, g, ψ) of equations [1]–[2] is via the initial-value (or Cauchy) formulation. The idea is as follows:

1. One chooses a set of initial data \mathcal{D} which consists of geometric as well as matter information on a spacelike slice of M^4 . This data must satisfy a system of constraint equations, which comprise a portion of the field equations [1]–[2], and are analogous to the Maxwell constraint equation $\nabla \cdot E = 0$.
2. One fixes a time and coordinate choice to be used in evolving the fields into the spacetime (e.g., maximal time slicing and zero shift). This choice should result in a fixed set of evolution equations for the data.
3. Using the evolution equations, one evolves the data into the future and the past. From the evolved data, one constructs the spacetime solution (M^4, g, ψ) .

Why is this procedure so popular? First, because we have known for over 50 years that at least for a short time, it works. That is, as shown by Choquet-Bruhat (Foures-Bruhat 1952), the Cauchy

formulation is well posed. Second, because it fits with the way we like to model physical systems. That is, we first specify what the system is like now, and we then use the equations to determine the behavior of the system as it evolves into the future (or the past). Third, because the formulation is eminently amenable to numerical treatment. Indeed, virtually all numerical simulations of colliding black hole systems as well as of most other relativistic astrophysical systems are done using some version of the initial-value formulation. Finally, because the initial-value formulation casts the Einstein equations into a form which is readily accessible to many of the tools of geometric analysis. Questions such as cosmic censorship are turned into conjectures which can be analyzed and proved mathematically, and the proofs of both the positivity of mass and the Penrose mass inequality rely on an initial-value interpretation.

There are of course drawbacks to the Cauchy formulation. Foremost, Einstein's theory of general relativity is inherently a spacetime-covariant theory; why break spacetime apart into space plus time when covariance has played such a key role in the theory's success? As well, we have learned over and over again that null cones and null hypersurfaces play a major role in general relativity; the initial-value formulation is not especially good at handling them. These drawbacks show that there are analyses in general relativity for which the initial-value formulation may not be well suited. However, there is a preponderance of applications for which this formulation is an invaluable tool, as evidenced by its ubiquitous use.

A complete treatment of the initial-value formulation for Einstein's equations would include discussion of each of the following topics:

1. A statement and proof of well-posedness theorems, including a discussion of the regularity of the data needed for such results.
2. A space + time decomposition of the fields, and a formal derivation of the Einstein constraint equations and the Einstein evolution equations.

3. An outline of the Hamiltonian version of the initial-value formulation.
4. A listing of those choices of field variables and gauge choices for which the system is manifestly hyperbolic.
5. A description of the known methods for finding and parametrizing solutions of the Einstein constraint equations.
6. A comparison of the virtues and drawbacks of various choices of time foliation and coordinate threading.
7. A compendium of results concerning long-time behavior of solutions.
8. An account of the difficulties which arise in attempts to construct solutions numerically using the Cauchy formulation.
9. A recounting of cases in which the initial-value formulation has been used to model physically interesting systems.
10. A note regarding the extent to which the initial-value formulation (and the various aspects of it just enumerated) generalize to dimensions other than $3 + 1$ (three space and one time).
11. A determination of which nongravitational fields may be coupled to Einstein's theory in such a way that the resulting coupled theory admits an initial-value formulation.

We do not have the space here for such a complete treatment. So we choose to focus on those topics directly related to the Einstein constraint equations. Generalizing a bit to the Einstein–Maxwell theory (thereby including representative nongravitational fields), we first carry out the space plus time “ $3 + 1$ ” decomposition of the gravitational and electromagnetic fields. Then, applying the Gauss–Codazzi–Mainardi equations to the spacetime curvature, we turn the spacetime-covariant Einstein–Maxwell equations into a set of constraint equations restricting the choice of initial data together with a set of evolution equations developing the data in time. Next, we discuss the most widely used approach for obtaining sets of initial data which satisfy the constraint equations: the conformal method. We include in this discussion an account of some of what is known about the extent to which the equations which are produced by the conformal method admit solutions in various situations (e.g., working on a closed manifold, or working with asymptotically Euclidean data). We then discuss alternate procedures which have been used to obtain and analyze solutions of the constraints, including the conformal thin sandwich approach, the quasispherical method, and various gluing procedures. Finally, we make concluding

remarks. For more details on some of the topics discussed here, and for treatment of some of the other topics listed above, see the recent review paper of Bartnik and Isenberg (2004).

Space + Time Field Decomposition and Derivation of the Constraint Equations

To understand what sort of initial data one needs to choose in order to construct a spacetime via the initial-value formulation, it is useful to consider a spacetime (M^4, g) which satisfies the Einstein (–Maxwell) field equations and contains a Cauchy surface $i_0: \Sigma^3 \rightarrow M^4$. We note that the existence of a Cauchy surface in (M^4, g, A) is not automatic; if one exists, the spacetime is said to be (by definition) “globally hyperbolic.”¹

Among its other properties, a Cauchy surface is a spacelike embedded submanifold of a Lorentz geometry. It immediately follows that the spacetime (M^4, g, A) induces on Σ^3 a Riemannian metric γ , a timelike normal vector field e_\perp , an intrinsic (γ -compatible) covariant derivative ∇ , and a symmetric “extrinsic curvature” tensor field K (second fundamental form). It also follows that certain components of the spacetime curvature tensor can be written in terms of these Cauchy surface quantities $(\gamma, e_\perp, \nabla, K)$ along with other geometric quantities related to them, such as the spatial curvature R corresponding to the induced covariant derivative ∇ (Gauss–Codazzi equations).

To complete the curvature $3 + 1$ decomposition (i.e., to carry it out for all components of the spacetime curvature), we need not just one Cauchy surface, but rather a full local foliation $i_t: \Sigma^3 \rightarrow M^4$ of the spacetime by such submanifolds. This foliation allows one to define e_\perp as a smooth vector field on an open neighborhood of the Cauchy surface $i_0(\Sigma^3)$ in M^4 . It also results in a threading of spacetime by a congruence of timelike paths (see Figure 1). This threading may be viewed as a spacetime-filling family of observers. It also defines for the spacetime a set of coordinates relative to which one can measure and calculate the dynamics of the spacetime geometry.

It is useful for later purposes to note that at each spacetime point $p \in \Sigma_t \subset M^4$ (Here $\Sigma_t := i_t(\Sigma^3)$.) the vector $\partial/\partial t$ tangent to the threading path through p may be decomposed as

$$\frac{\partial}{\partial t} = N e_\perp + X \quad [3]$$

¹The Taub–NUT spacetime is an example of a spacetime which is *not* globally hyperbolic.

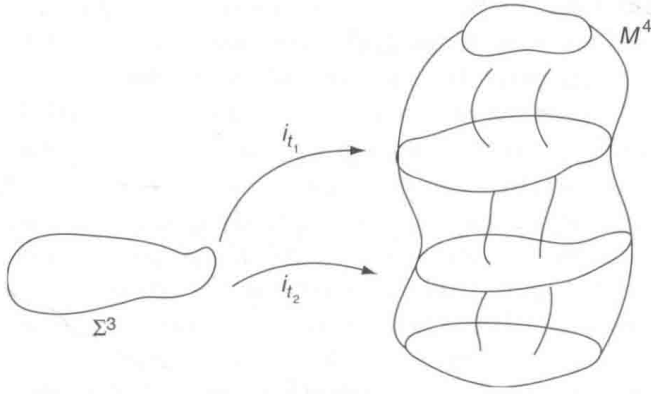


Figure 1 3 + 1 Foliation and threading of spacetime.

with the “shift vector” X tangent to the surface ($X \in T_p \Sigma_t$), and with the “lapse” N a scalar (see Figure 2). Using these quantities, we can write the spacetime metric in the form

$$g = \gamma - \theta^\perp \otimes \theta^\perp \\ = \gamma_{ab}(dx^a + X^a dt)(dx^b + X^b dt) - N^2 dt^2 \quad [4]$$

where θ^\perp is the unit length timelike 1-form which annihilates all vectors tangent to the hypersurfaces of the foliation.

Relying on the following 3 + 1 decomposition of the spacetime-covariant derivative ${}^4\nabla$ (Here $\{\partial_a\}$ is a coordinate basis for the vectors tangent to the hypersurfaces of the foliation; $\{\partial_a, e_\perp\}$ constitutes a basis for the full set of spacetime vectors at p):

$${}^4\nabla_{\partial_a} \partial_b = \nabla_{\partial_a} \partial_b - K_{ab} e_\perp \quad [5]$$

$${}^4\nabla_{\partial_a} e_\perp = -K_a^m \partial_m \quad [6]$$

$${}^4\nabla_{e_\perp} \partial_b = -K_b^m \partial_m + [e_\perp, \partial_b] + \frac{\partial_b N}{N} e_\perp \quad [7]$$

$${}^4\nabla_{e_\perp} e_\perp = \gamma^{mn} \frac{\partial_m N}{N} \partial_n \quad [8]$$

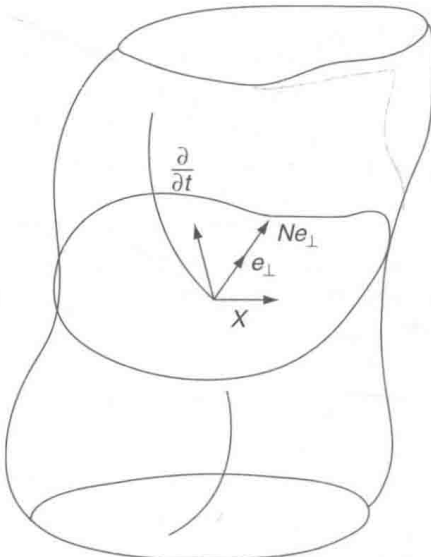


Figure 2 Decomposition of the time evolution vector field $\partial/\partial t$.

one readily derives the (Gauss–Codazzi–Mainardi) 3 + 1 decomposition of the curvature:²

$${}^4R_{abc}^e = R_{abc}^e + K_{ac}K_b^e - K_{ab}K_c^e \quad [9]$$

$${}^4R_{abc}^\perp = \nabla_{\partial_c} K_{ab} - \nabla_{\partial_b} K_{ac} \quad [10]$$

$${}^4R_{a\perp b}^\perp = -\mathcal{L}_{e_\perp} K_{ab} - K_{am}K_b^m + \frac{\nabla_{\partial_a} \nabla_{\partial_b} N}{N} \quad [11]$$

where \mathcal{L} denotes the surface-projected Lie derivative.

Since we are interested here in the 3 + 1 formulation of the Einstein–Maxwell system, we need a 3 + 1 decomposition for the electromagnetic as well as the gravitational field. The spacetime 1-form “vector potential” 4A pulls back on each Cauchy surface Σ_t to a spatial 1-form A . One may then write

$${}^4A = A + \mu \theta^\perp = A_b dx^b + (N\mu + A_b X^b) dt \quad [12]$$

for a scalar μ . Based on this decomposition, one has the following 3 + 1 decomposition for the electromagnetic 2-form F :

$${}^4F_{\perp a} = \gamma_{ac} E^c \quad [13]$$

$${}^4F_{ab} = \nabla_{\partial_a} A_b - \nabla_{\partial_b} A_a \quad [14]$$

where E^c is the electric vector field.

We may now use all of these decomposition formulas to write out the 14 field equations for the Einstein–Maxwell theory

$${}^4G_{\alpha\beta} = F_\alpha^\mu F_{\beta\mu} - \frac{1}{4} g_{\alpha\beta} F^{\mu\nu} F_{\mu\nu} \quad [15]$$

$${}^4\nabla_\mu ({}^4F_\alpha^\mu) = 0 \quad [16]$$

in terms of the spatial fields $(\gamma, K, N, X; A, E, \mu)$ and their derivatives. We obtain

$$R - K^{mn} K_{mn} + (\text{tr } K)^2 = \frac{1}{2} E^m E_m + \frac{1}{2} B^m B_m \quad [17]$$

$$\nabla_m K_a^m - \nabla_{\partial_a} (\text{tr } K) = \epsilon_{amn} E^m B^n \quad [18]$$

$$\mathcal{L}_{e_\perp} K_{ab} = R_{ab} - 2K_a^m K_{mb} + (\text{tr } K) K_{ab} \\ + E_a E_b + B_a B_b - \frac{\nabla_{\partial_a} \nabla_{\partial_b} N}{N} \quad [19]$$

$$\nabla_{\partial_m} E^m = 0 \quad [20]$$

$$\mathcal{L}_{e_\perp} E^a = \epsilon^{amn} \nabla_{\partial_m} B_n \quad [21]$$

where ϵ_{abc} is the alternating Levi-Civita symbol (component representation of the Hodge dual), and where we have used $B_a := \epsilon_a^{mn} (\nabla_{\partial_m} A_n - \nabla_{\partial_n} A_m)$ as a convenient shorthand.

²Here and throughout this article, we use the Misner–Thorne–Wheeler (MTW) (Misner *et al.* 1973) conventions for the definition of the Riemann curvature, for the signature $-+++$ of the metric, for the index labels (Greek indices run over $\{0, 1, 2, 3\}$ while Latin indices run over $\{1, 2, 3\}$), etc.

It is immediately evident that nine of these equations ([19] and [21]) involve time derivatives of the spatial fields, while five of them ([17], [18], and [20]) do not. Thus, we may split the field equations of the Einstein–Maxwell theory into two sets: (1) the constraint equations [17], [18], and [20], which restrict our choice of the Einstein–Maxwell initial data (γ, K, A, E) ; and (2) the evolution equations, which describe how to evolve the data (γ, K, A, E) in time, presuming that one has also prescribed (freely!) the “atlas fields” (N, X, μ) .³ We note that the complete system of evolution equations for the Einstein–Maxwell field equations includes equations which are based on the definitions of K and E . Written in terms of (surface-projected) Lie derivatives along $\partial/\partial t$, the full system takes the form

$$\mathcal{L}_{\frac{\partial}{\partial t}}\gamma_{ab} = -2NK_{ab} + \mathcal{L}_X\gamma_{ab} \quad [22]$$

$$\mathcal{L}_{\frac{\partial}{\partial t}}K_{ab} = N(R_{ab} - 2K_a^m K_{mb} + K_m^m K_{ab} + E_a E_b + B_a B_b) - \nabla_{\partial_a}\nabla_{\partial_b}N + \mathcal{L}_X K_{ab} \quad [23]$$

$$\mathcal{L}_{\frac{\partial}{\partial t}}A_a = N(E_a + \nabla_{\partial_a}\mu) + \mathcal{L}_X A_a \quad [24]$$

$$\mathcal{L}_{\frac{\partial}{\partial t}}E^a = N\epsilon^{amn}\nabla_{\partial_m}B_n + \mathcal{L}_X E^a \quad [25]$$

As noted earlier, well-posedness theorems⁴ guarantee that initial data satisfying the constraint equations [17], [18], and [20] on a manifold Σ^3 can always at least locally be evolved into a spacetime solution $(\Sigma^3 \times I, g, {}^4A)$ (for I some interval in R^1) of the Einstein–Maxwell equations. We now turn our attention to the issue of finding sets of data which do satisfy the constraints.

The Conformal Method

We seek to find sets of data (γ, K, A, E) on a manifold Σ^3 which satisfy the constraint equations

$$R - K^{mn}K_{mn} + (\text{tr } K)^2 = \frac{1}{2}E^m E_m + \frac{1}{2}B^m B_m \quad [26]$$

$$\nabla_m K_a^m - \nabla_a(\text{tr } K) = \epsilon_{amn}E^m B^n \quad [27]$$

$$\nabla_m E^m = 0 \quad [28]$$

³The collective name “atlas field” for the lapse N , the shift X , the electric potential μ , and other such fields which are neither constrained by the constraint equations nor evolved by the evolution equations, derives from their role in controlling the evolution of coordinate charts and bundle atlases in the course of the construction of spacetime solutions of relativistic field equations like the Einstein–Maxwell system.

⁴While the work cited earlier (Foures-Bruhat 1952) proves well posedness for the vacuum Einstein equations only, the extension to the Einstein–Maxwell system is straightforward

(Here and below, for convenience, we replace ∇_{∂_a} by ∇_a .) This is an underdetermined problem, with five equations to be solved for 18 functions.

The idea of the conformal method is to divide the initial data on Σ^3 into two sets – the “free (conformal) data,” and the “determined data” – in such a way that, for a given choice of the free data, the constraint equations become a determined elliptic partial differential equation (PDE) system, to be solved for the determined data. There are a number of ways to do this; we focus here on one of them – the “semidecoupling split” or “method A.” After describing this version of the conformal method, and discussing what one can do with it, we note some of its drawbacks and then later (in the next section) consider some alternatives. (See Choquet-Bruhat and York (1980) and Bartnik and Isenberg (2004) for a more complete discussion of these alternatives.)

For the Einstein–Maxwell theory, the split of the initial data is as follows:

Free (“conformal”) data

λ_{ij} – a Riemannian metric, specified up to conformal factor;

σ_{ij} – a divergence-free⁵ ($\nabla^i \sigma_{ij} = 0$), tracefree ($\lambda^{ij}\sigma_{ij} = 0$); symmetric tensor;

τ – a scalar field;

α_a – a 1-form;

\mathcal{E}^b – a divergence-free vector field;

Determined data

ϕ – a positive-definite scalar field;

W^i – a vector field;

ξ – a scalar field.

For a given choice of the free data, the five equations to be solved for the five functions of the determined data take the form

$$\Delta\xi = 0 \quad [29]$$

$$\nabla_m(LW)^m_a = \frac{2}{3}\phi^6\nabla_{\partial_a}\tau + \epsilon_{amn}\mathcal{E}^m\beta^n \quad [30]$$

$$\Delta\phi = \frac{1}{8}R\phi - \frac{1}{8}(\sigma^{mn} + LW^{mn})(\sigma_{mn} + LW_{mn})\phi^{-7} + \frac{1}{16}(\mathcal{E}^m\mathcal{E}_m + \beta^m\beta_m)\phi^{-3} + \frac{1}{12}\tau^2(\phi^5) \quad [31]$$

where the Laplacian Δ and the scalar curvature R are based on the λ_{ab} -compatible covariant derivative ∇_i , where L is the corresponding conformal Killing operator, defined by

$$(LW)_{ab} := \nabla_a W_b + \nabla_b W_a - \frac{2}{3}\lambda_{ab}\nabla_m W^m \quad [32]$$

⁵In the free data, the divergence-free condition is defined using the Levi-Civita-covariant derivative compatible with the conformal metric λ_{ij} .

and where $\beta_a := \epsilon_a^{mn}(\nabla_{\partial_m} \alpha_n - \nabla_{\partial_n} \alpha_m)$. Presuming that for the chosen free data one can indeed solve equations [29]–[31] for ξ, ϕ , and W , then the initial data (γ, K, A, E) constructed via the formulas

$$\gamma_{ab} = \phi^4 \lambda_{ab} \quad [33]$$

$$K_{ab} = \phi^{-2}(\sigma_{ab} + L W_{ab}) + \frac{1}{3} \phi^4 \lambda_{ab} \tau \quad [34]$$

$$A_b = \alpha_b \quad [35]$$

$$E^a = \phi^{-6}(\mathcal{E}_a + \nabla_{\partial a} \xi) \quad [36]$$

satisfy the Einstein–Maxwell constraint equations [26]–[28].

Before discussing the extent to which one can solve equations [29]–[31] and consequently use the conformal method to generate solutions, we wish to comment on how these equations are derived. Three formulas are key to this derivation. The first is the formula for the scalar curvature of the metric $\gamma_{ab} = \phi^4 \lambda_{ab}$, expressed in terms of the scalar curvature for λ_{ab} and derivatives of ϕ :

$$R(\gamma) = \phi^{-4} R(\lambda) - 8 \Delta_\lambda \phi \quad [37]$$

We note that if we were to use a different power of ϕ as the conformal factor multiplying λ_{ab} , then this formula would involve squares of first derivatives of ϕ as well. The second key formula relates the divergence of a traceless symmetric tensor ρ_{ab} with respect to the covariant derivatives $\nabla_{(\gamma)}$ and $\nabla_{(\lambda)}$ compatible with conformally related metrics. One obtains

$$\nabla_{(\gamma)}^m \rho_{mb} = \phi^{-2} \nabla_{(\lambda)}^m (\phi^2 \rho_{mb}) \quad [38]$$

The third key formula does the same thing for a vector field ζ^a :

$$\nabla_{(\gamma)m} \zeta^m = \phi^{-6} \nabla_{(\lambda)}^m (\phi^6 \zeta_m) \quad [39]$$

In addition to helping us derive equations [29]–[31] from the substitution of formulas [33]–[36] into [26]–[28], these key formulas indicate to some extent how the choice of the explicit decomposition of the initial data into free and determined data is made (see Isenberg, Maxwell, and Pollack for further elaboration).

It is easy to see that there are some choices of the free data for which [29]–[31] do not admit any solutions. Let us choose, for example, Σ^3 to be the 3-sphere, and let us set λ to be the round sphere metric, σ to be zero everywhere, τ to be unity everywhere, and both α and \mathcal{E} to vanish everywhere. We then readily determine that eqn [29] requires that ξ be constant and that eqn [30] requires that LW_{ab} be zero. The remaining equation [31] now takes the form $\Delta\phi = (1/8)R\phi + (1/12)\phi^5$. Since the

right-hand side of this equation is positive definite (recall the requirement that $\phi > 0$), it follows from the maximum principle on closed (compact without boundary) manifolds that there is no solution.

In light of this example, one would like to know exactly for which sets of free data eqns [29]–[31] can be solved, and for which sets they cannot. Since one readily determines that every set of initial data which satisfies the Einstein–Maxwell constraints [26]–[28] can be obtained via the conformal method, such a classification effectively provides a parametrization of the space of solutions of the constraints.⁶

What we know and do not know about classifying free data for the solubility of eqns [29]–[31] is largely determined by whether or not the function τ is chosen to be constant on Σ^3 . If τ is chosen to be constant, then eqns [29]–[31] effectively decouple, and the classification is essentially completely known. Sets of initial data generated from free data with constant τ are called “constant mean curvature” (CMC) sets, since the mean curvature of the initial slice embedded in its spacetime development is given by τ . We also know a considerable amount about the classification if $|\nabla\tau|$ is sufficiently small (“near CMC”), while virtually nothing is known for the general non-CMC case.

A full account of the classification results known to date is beyond the scope of this article. Indeed, such an account must separately deal with a number of alternatives regarding manifold and asymptotic conditions (data on a closed manifold; asymptotically Euclidean data; asymptotically hyperbolic data; data on an incomplete manifold with boundaries) and regularity (analytic data, smooth data, C^k data, or data contained in various Hölder or Sobolev spaces), among other things. We will, however, now summarize some of the results; see, for example, Bartnik and Isenberg (2004) or Choquet-Bruhat for more complete surveys.

CMC Data on Closed Manifolds

Generalizing the S^3 example given above, we note that for any set of free data $(\Sigma^3, \lambda_{ab}, \sigma_{ab}, \tau, \alpha_a, \mathcal{E}^b)$ with constant τ and with no conformal Killing fields, eqn [29] is easily solved for ξ , and then eqn [30] takes the form

$$\nabla_m (LW)_a^m = \epsilon_{amn} \mathcal{E}^m \beta^n \quad [40]$$

⁶Of course, in claiming that appropriate sets of the free data parametrize the space of solutions of the constraints, one needs to determine if inequivalent sets of free data are mapped to the same set of solutions. We discuss this below.

which is a linear elliptic PDE for W_m with invertible operator.⁷ This equation admits a unique solution, and then the problem of solving the constraints reduces to the analysis of the “Lichnerowicz equation” [31].

To determine if this equation admits a solution for the given set of free data, we use the following classification criteria: (1) The metric is labeled positive $\mathcal{Y}^+(\Sigma^3)$, zero $\mathcal{Y}^0(\Sigma^3)$, or negative $\mathcal{Y}^-(\Sigma^3)$ Yamabe class depending upon whether the metric λ_{ab} on Σ^3 can be conformally deformed so that its scalar curvature is everywhere positive, everywhere zero, or everywhere negative.⁸ (2) The $(\sigma_{ab}, \alpha_a, \mathcal{E}^b)$ portion of the data is labeled either \equiv or \neq , depending upon whether the quantity $\sigma_{mn}\sigma^{mn} + \mathcal{E}^m\mathcal{E}_m + \beta^m\beta_m$ is identically zero, or not. (3) The mean curvature τ is labeled “max” or “nonmax” depending upon whether the constant τ is zero or not. In terms of these criteria, we have 12 classes of free data, and one can prove (Choquet-Bruhat and York 1980, Isenberg 1995) the following:

- Solutions exist for the classes $(\mathcal{Y}^+, \neq, \text{max})$, $(\mathcal{Y}^+, \neq, \text{nonmax})$, $(\mathcal{Y}^0, \equiv, \text{max})$, $(\mathcal{Y}^0, \neq, \text{max})$, $(\mathcal{Y}^-, \equiv, \text{nonmax})$, $(\mathcal{Y}^-, \neq, \text{nonmax})$ and
- Solutions do not exist for the classes $(\mathcal{Y}^+, \equiv, \text{max})$, $(\mathcal{Y}^+, \equiv, \text{nonmax})$, $(\mathcal{Y}^0, \equiv, \text{nonmax})$, $(\mathcal{Y}^0, \neq, \text{max})$, $(\mathcal{Y}^-, \equiv, \text{max})$, $(\mathcal{Y}^-, \neq, \text{max})$.

This classification is exhaustive, in the sense that every set of CMC data on a closed manifold fits neatly into exactly one of the classes. We note that the proofs of existence of solutions can generally be done using the sub-super solution technique, while the nonexistence results follow from application of the maximum principle.

Maximal Asymptotically Euclidean Data

Just as is the case for data on a closed manifold, the constraint equations [29] and [30] decouple from the Lichnerowicz equation [31] for asymptotically Euclidean data with constant τ . We note that $\tau \neq 0$ is inconsistent with the data being

asymptotically Euclidean, so we restrict to the maximal case, $\tau = 0$.

The criterion for solubility of the constraints in conformal form for maximal asymptotically Euclidean free data is quite a bit simpler to state than that for CMC data on a closed manifold. It involves the metric λ only; the rest of the free data is irrelevant. Specifically, as shown by Brill and Cantor (with a correction by Maxwell (2005)), a solution exists if and only if for every nonvanishing, compactly supported, smooth function f on Σ^3 , we have

$$\inf_{\{f \neq 0\}} \frac{\int_M (|\nabla f|^2 + Rf^2) \sqrt{\det \lambda}}{\|f\|_{L^2}^2} > 0 \quad [41]$$

Alternative Methods for Finding Solutions to the Constraint Equations

While the conformal method has proved to be a very useful tool for generating and analyzing solutions of the Einstein constraint equations, it does have some minor drawbacks: (1) The free data is remote from the physical data, since the conformal factor can vastly change the physical scale on different regions of space. (2) While casting the constraints into a determined PDE form has the advantage of producing PDEs of a relatively familiar (elliptic) form, one does give up certain flexibilities inherent in an underdetermined set of PDEs. (We expand upon this point below in the course of discussing gluing.). (3) In choosing a set of free data, one does have to first project out a divergence-free vector field (\mathcal{E}) and a divergence-free tracefree tensor field (σ). (4) While the choice of CMC free data for the conformal method is conformally covariant in the sense that conformally related sets of CMC free data $(\Sigma^3, \lambda_{ab}, \sigma_{ab}, \tau, \alpha_a, \mathcal{E}^b)$ and $(\Sigma^3, \theta^4 \lambda_{ab}, \theta^{-2} \sigma_{ab}, \tau, \alpha_a, \theta^{-6} \mathcal{E}^b)$ produce the same physical solution to the constraints, this is not the case for non-CMC free data.

Conformal Thin Sandwich

The last two of these problems can be removed by modifying the conformal method in a way which York (1999) has called the “conformal thin sandwich” (CTS) approach. The basic idea of the CTS approach is the same as that of the conformal method. However, CTS free data sets are larger – the divergence-free tracefree symmetric tensor field σ is replaced by a tracefree symmetric tensor field U ,

⁷A metric λ has a conformal Killing field if the equation $LY=0$ has a nontrivial solution Y . Geometrically, the existence of a conformal Killing field Y indicates that the flow of (Σ^3, λ_{ab}) along Y is a conformal isometry. While free data with nonvanishing conformal Killing fields can be handled, for convenience we shall stick to data without them here.

⁸Work on the Yamabe problem (Aubin 1998) shows that every Riemannian metric on a closed manifold is contained in one and only one of these classes. In fact, the Yamabe theorem (Schoen 1984) shows that every metric can be conformally deformed so that its scalar curvature is $+1, 0$, or -1 , but this result is not needed for the analysis of the constraint equations.

and an extra scalar field η is added – and after solving the CTS constraint equations

$$\Delta\xi = 0 \quad [42]$$

$$\begin{aligned} \nabla_m((2\eta)^{-1}(LX))_a^m &= \frac{2}{3}\Phi^6\nabla_a\tau + \epsilon_{amn}\mathcal{E}^m\beta^n \\ &+ \nabla_m((2\eta)^{-1}U_a^m) \end{aligned} \quad [43]$$

$$\begin{aligned} \Delta\Phi &= \frac{1}{8}R\Phi - \frac{1}{8}(U^{mn} + LY^{mn})(U_{mn} + LY_{mn})\Phi^{-7} \\ &+ \frac{1}{16}(\mathcal{E}^m\mathcal{E}_m + \beta^m\beta_m)\Phi^{-3} + \frac{1}{12}\tau^2\Phi^5 \end{aligned} \quad [44]$$

for the vector field Y and the conformal factor Φ , one obtains not just the full set of physical initial data satisfying the constraint equations [26]–[28]

$$\gamma_{ab} = \phi^4\lambda_{ab} \quad [45]$$

$$K_{ab} = \Phi^{-2}(-U_{ab} + LY_{ab}) + \frac{1}{3}\Phi^4\lambda_{ab}\tau \quad [46]$$

$$A_b = \alpha_b \quad [47]$$

$$E^a = \Phi^{-6}(\mathcal{E}_a + \nabla_a\xi) \quad [48]$$

but also the lapse N and shift X

$$N = \Phi^6\eta \quad [49]$$

$$X^a = Y^a \quad [50]$$

Clearly, in using the CTS approach, one need not project out a divergence-free part of a symmetric tracefree tensor. One also readily checks that the CTS method is conformally covariant in the sense discussed above: the physical data generated from CTS free data $(\lambda_{ab}, U_{ab}, \tau, \eta, \alpha_a, \mathcal{E}^b)$ and from data $(\theta^4\lambda_{ab}, \theta^{-2}U_{ab}, \tau, \theta^6\eta, \alpha_a, \theta^{-6}\mathcal{E}^b)$ are the same. Furthermore, since the mathematical form of eqns [42]–[44] is very similar to that of [29]–[31], the solvability results for the conformal method can be essentially carried over to the CTS approach.

There is, however, one troubling feature of the CTS approach. The problem arises if we seek CMC initial data with the lapse function chosen so that the evolving data continue to have CMC (such a gauge choice is often used in numerical relativity). In the case of the conformal method, after solving [29]–[31] to obtain initial data $(\gamma_{ab}, K_{ab}, A_a, E^b)$ which satisfies the constraints, one achieves this by proceeding to solve a linear homogeneous elliptic PDE for the lapse function. One easily verifies that solutions to this extra equation always exist. By contrast, in the CTS approach, the extra equation takes the form

$$\begin{aligned} \Delta(\Phi^7\eta) &= \frac{1}{8}\Phi^7\eta R + \frac{5}{2}(\Phi\eta)^{-1}(U - LX)^2 \\ &+ \frac{1}{16}(\Phi\eta)^{-1}(\mathcal{E}^2 + \beta^2) \\ &+ \Phi^5 Y^m \nabla_{\partial_m} \tau - \Phi^5 \end{aligned} \quad [51]$$

which is coupled to the system [42]–[44]. The coupling is fairly intricate; hence little is known about the existence of solutions to the system, and it has been seen that there are problems with uniqueness. Such problems of course do not arise if one makes no attempt to preserve CMC.

The Quasispherical Ansatz and Parabolic Methods

Applying either the conformal method or the CTS approach to the constraint equations results in systems of elliptic equations. Another approach, pioneered by Bartnik (1993), produces instead parabolic equations. In the simplest version of this approach, known as the “quasispherical ansatz,” one works on a manifold $\Sigma^3 = R^3 \setminus B_3$, where B_3 is a 3-ball; one presumes that there exist coordinates (r, θ, ϕ) on Σ^3 in terms of which the metric takes the “quasispherical” form

$$\begin{aligned} \gamma_{QS} &= u^2 dr^2 + (r d\theta + \beta^\theta dr)^2 \\ &+ (r \sin \theta d\phi + \beta^\phi dr)^2 \end{aligned} \quad [52]$$

for functions $u(r, \theta, \phi)$, $\beta^\theta(r, \theta, \phi)$, $\beta^\phi(r, \theta, \phi)$, and then one attempts to satisfy the time-symmetric constraint $R_{(\gamma_{QS})} = 0$ on Σ^3 .⁹ Calculating the scalar curvature for the metric in this form, one finds that the equation $R_{(\gamma_{QS})} = 0$ can be written as

$$\begin{aligned} (r\partial_r - \beta^\theta\partial_\theta - \beta^\phi\partial_\phi)u - u^2\Delta u \\ = Q(u, \beta^\theta, \beta^\phi, r, \theta, \phi) \end{aligned} \quad [53]$$

where Q is a polynomial in the positive function u .

One can now show that if one specifies β^θ and β^ϕ everywhere on Σ^3 (subject to an upper bound on the divergence of the vector field $(\beta^\theta, \beta^\phi)$), and if one specifies regular initial data for u on the inner boundary of Σ^3 , then one has a well-posed initial-value problem (in terms of the “evolution” coordinate r) for the parabolic PDE [53]. Ideally, one can use this approach to extend solutions of the time-symmetric constraints from an isolated region (corresponding to B_3) out to spatial infinity.

The basic quasispherical ansatz approach just outlined can be generalized significantly (Sharples 2001, Bartnik and Isenberg 2004) to allow for more general spatial metrics, and to allow nonzero K_{ab} , A_c , and E^b . It has been an especially valuable tool for the study of mass in asymptotically Euclidean data sets. It does not, however, purport to construct general solutions of the constraint equations.

⁹This version of the constraints is called “time symmetric” since one is solving the full set of constraints with K_{ab} assumed to be zero. Data with $K_{ab} = 0$ is time symmetric.

Gluing Solutions of the Constraint Equations

Starting around the year 2000, a number of new “gluing” procedures have been developed for constructing and studying solutions of the constraint equations. Unlike the conformal method, the CTS method, and the quasispherical ansatz, all of which construct solutions from scratch, the gluing procedures construct new solutions from given ones. This feature, and the considerable flexibility of the procedures, has resulted in a wealth of applications already in the short five-year history of gluing in general relativity.

One of the gluing approaches, developed by Corvino (2000) and Corvino and Schoen (preprint) (see also Chruściel and Delay (2002)), allows one to choose a compact region Ω in almost any smooth, asymptotically Euclidean vacuum solution of the constraints, and from this produce a new smooth solution which is completely unchanged in the region Ω and is identical to Schwarzschild or Kerr outside some larger region. In proving this result, one exploits the underdetermined character of the constraint equations: such a construction could not be carried out if the constraints were a determined PDE system.¹⁰

The other main gluing approach, developed first by Isenberg *et al.* (2001), and then further developed with Chruściel (Chruściel *et al.* 2005) and with Maxwell (Isenberg *et al.* 2005), starts with a pair of solutions of the (vacuum) constraints $(\Sigma_1^3, \gamma_1, K_1)$ and $(\Sigma_2^3, \gamma_2, K_2)$ together with a choice of a pair of points $p_1 \in \Sigma_1^3$, $p_2 \in \Sigma_2^3$, one from each solution. From these solutions, this gluing procedure produces a new set of initial data $(\Sigma_{(1-2)}^3, \gamma_{(1-2)}, K_{(1-2)})$ with the following properties: (1) $\Sigma_{(1-2)}^3$ is diffeomorphic to the connected sum $\Sigma_1^3 \# \Sigma_2^3$; (2) $(\Sigma_{(1-2)}^3, \gamma_{(1-2)}, K_{(1-2)})$ is a solution of the constraints everywhere on $\Sigma_{(1-2)}^3$; (3) On that portion of $\Sigma_{(1-2)}^3$ which corresponds to $\Sigma_1^3 \setminus \{\text{ball around } p_1\}$, the data $(\gamma_{(1-2)}, K_{(1-2)})$ is isomorphic to (γ_1, K_1) , with a corresponding property holding on that portion of Σ_2^3 which corresponds to $\Sigma_2^3 \setminus \{\text{ball around } p_2\}$ (see Figure 3).¹¹

This connected sum gluing can be carried out for very general sets of initial data. The sets can be asymptotically Euclidean, asymptotically hyperbolic, specified on a closed manifold, or indeed anything

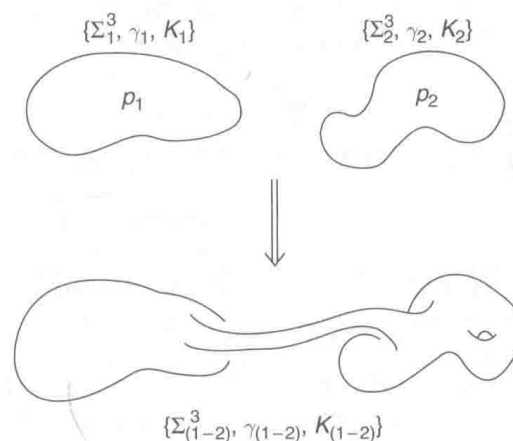


Figure 3 Connected sum gluing.

else. The only condition that the data sets must satisfy is that, in sufficiently small neighborhoods of each of the points at which the gluing is to be done, there do not exist nontrivial solutions ξ to the equation $D\Theta_{(\gamma, K)}^* \xi = 0$, where $D\Theta_{(\gamma, K)}^*$ is the operator obtained by taking the adjoint of the linearized constraint operator.¹² In work by Beig, Chruściel, and Schoen, it is shown that this condition (sometimes referred to as “No KIDs,” meaning “no (localized) Killing initial data”) is indeed generically satisfied.

While a discussion of the proof that connected sum gluing can be carried out to this degree of generality is beyond the scope of this paper (see Chruściel *et al.* (2005), along with references cited therein for details of the proof), we note three features of it: first, the proof is constructive in the sense that it outlines a systematic, step-by-step mathematical procedure for doing the gluing. In principle, one should be able to carry out the gluing procedure numerically. Second, connected sum gluing relies primarily on the conformal method, but it also uses a nonconformal deformation at the end (dependent on the techniques of Corvino and Schoen, and of Chruściel and Delay), so as to guarantee that the glued data is not just very close to the given data on regions away from the bridge, but is indeed identical to it. Third, while Corvino–Schoen gluing has not yet been proved to work for solutions of the constraints with source fields, connected sum gluing (up to the last step, which relies on Corvino–Schoen) has been shown to work for most matter source fields of interest (Isenberg *et al.*). It has also been shown to work for general dimensions greater than or equal to three.

¹⁰Hence if one tries to do Corvino–Schoen-type gluing using a fixed conformal geometry, the gluing fails because the determined elliptic system satisfies the unique continuation property.

¹¹The connected sum of the two manifolds (see property (1)) is constructed as follows: first we remove a ball from each of the manifolds Σ_1^3 and Σ_2^3 . We then use a cylindrical bridge $S^2 \times I$ (where I is an interval in \mathbb{R}^1) to connect the resulting S^2 boundaries on each manifold.

¹²When a solution to this equation does exist on some region $\Lambda \in \Sigma^3$, it follows from the work of Moncrief that the spacetime development of the data on Λ admits a nontrivial isometry.

While gluing is not an efficient tool for studying the complete set of solutions to the constraints, it has proved to be very valuable for a number of applications. We note a few here.

1. *Spacetimes with regular asymptotic structure.* Until recently, it was not known whether there is a large class of solutions which admit the conformal compactification and consequent asymptotically simple structure at null and space-like infinity characteristic of the Minkowski and Schwarzschild spacetimes. Using Corvino–Schoen gluing, together with Friedrich’s analyses of spacetime asymptotic structures and an argument of Chruściel and Delay (2002), one produces such a class of solutions.
2. *Multi-black hole data sets.* Given an asymptotically Euclidean solution of the constraints, connected sum gluing allows a sequence of (almost) flat space initial data sets to be glued to it. The bridges that result from this gluing each contain a minimal surface, and consequently an apparent horizon. With a bit of care, one can do this in such a way that indeed the event horizons which appear in the development of this glued data are disjoint, and therefore indicative of independent black holes.
3. *Adding a black hole to a cosmological spacetime.* Although there is no clear established definition for a black hole in a spatially compact solution of Einstein’s equations, one can glue an asymptotically Euclidean solution of the constraints to a solution on a compact manifold, in such a way that there is an apparent horizon on the bridge. Studying the nature of these solutions of the constraints, and their evolution, could be useful in trying to understand what one might mean by a black hole in a cosmological spacetime.
4. *Adding a wormhole to your spacetime.* While we have discussed connected sum gluing as a procedure which builds solutions of the constraints with a bridge connecting two points on different manifolds, it can also be used to build a solution with a bridge connecting a pair of points on the same manifold. This allows one to do the following: if one has a globally hyperbolic spacetime solution of Einstein’s equations, one can choose a Cauchy surface for that solution, choose a pair of points on that Cauchy surface, and glue the solution to itself via a bridge from one of these points to the other. If one now evolves this glued-together initial data into a spacetime, it will likely become singular very quickly because of the collapse of the bridge. Until the singularity develops, however, the solution is essentially as it was before the gluing,

with the addition of an effective wormhole. Hence, this procedure can be used to glue a wormhole onto a generic spacetime solution.

5. *Removing topological obstructions for constraint solutions.* We know that every closed three-dimensional manifold M^3 admits a solution of the vacuum constraint equations. To show this, we use the fact that M^3 always admits a metric Γ of constant negative scalar curvature. One easily verifies that the data $(\gamma = \Gamma, K = \Gamma)$ is a CMC solution. Combining this result with connected sum gluing, one can show that for every closed Σ^3 , the manifold $\Sigma^3 \setminus \{p\}$ admits both an asymptotically Euclidean and an asymptotically hyperbolic solution of the vacuum constraint equations.
6. *Proving the existence of vacuum solutions on closed manifolds with no CMC Cauchy surface.* Based on the work of Bartnik (1988) one can show that if one has a set of initial data on the manifold $T^3 \# T^3$ with the metric components symmetric across a central sphere and the components of K skew symmetric across that same central sphere, then the spacetime development of that data does not admit a CMC Cauchy surface. Using connected sum gluing, one can show that indeed initial data sets of this sort exist (Chruściel *et al.* 2005).

Conclusion

Much is known about the Einstein constraint equations and those sets of initial data which satisfy them. We know how to use the conformal method or the CTS approach to construct (and parametrize in terms of free data) the CMC and near CMC sets of data which solve the constraints, with or without matter fields present. We know how to use the quasispherical approach to explore extensions of solutions of the constraint equations from compact regions. We know how to use gluing techniques to produce new solutions of both physical and mathematical interest from old ones, and we know how to use gluing as a tool for proving such results as the existence of vacuum spacetimes with no CMC Cauchy surfaces.

There is much that is not yet known as well. Very little is known about solutions of the constraint equations which have neither CMC nor near CMC. It is not known how to systematically extend solutions of the constraints from a compact region to all of R^3 in such a way that the extension is asymptotically Euclidean (unless we know *a priori* that such an extension exists). Very little is known regarding how to control the constraints during the course of

numerical evolution of solutions.¹³ Most importantly, we do not yet know how to systematically find solutions of the constraint equations which serve as physically realistic model initial data sets for studying astrophysical and cosmological systems of interest.

Many of these questions concerning the Einstein constraints and their solutions are fairly daunting. However, in view of the rapid progress in our understanding during the last few years, and in view of the pressing need to further develop the initial-value formulation as a tool for studying general relativity and gravitational physics, we are optimistic that this progress will continue, and we will soon have answers to a number of these questions.

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See also: Asymptotic Structure and Conformal Infinity; Computational Methods in General Relativity: The Theory; Dirac Fields in Gravitation and Nonabelian Gauge Theory; Einstein Manifolds; Einstein's Equations with Matter; General Relativity: Overview; Geometric Analysis and General Relativity; Hamiltonian Reduction of Einstein's Equations; Spacetime Topology, Causal Structure and Singularities; Stationary Black Holes; Symmetric Hyperbolic Systems and Shock Waves.

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¹³If the constraints are satisfied by an initial data set and if this data set is evolved completely accurately, then the constraints remain satisfied for all time. However, during the course of a numerical evolution, there are inevitable numerical inaccuracies which result in the constraints not being exactly zero. In practice, during the majority of such numerical simulations to date, the constraints have been seen to increase very rapidly in time, calling into question the reliability of the simulation.

Einstein Manifolds

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Introduction

The Einstein condition on a manifold M with metric g says that the Ricci curvature should be proportional to the metric. Of course, this condition

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originally appeared in relativity, but it is of tremendous interest from the point of view of pure mathematics. Demanding a metric of constant sectional curvature is a very strong condition, while metrics of constant scalar curvature always occur. The Einstein property, which is essentially a constant-Ricci-curvature condition, occupies an intermediate position between these conditions, and it is still not clear exactly how strong it is. In

dimensions higher than four, it is still unknown whether there are obstructions to a manifold admitting an Einstein metric.

The study of Einstein manifolds is a vast and rapidly expanding area, and this article can merely touch on some points of particular interest. The focus of the article is very much on the Riemannian rather than Lorentzian case (see, e.g., Hawking and Ellis (1973) or the articles by Christodoulou and Tod in LeBrun and Wang (1999) for a discussion of the Lorentzian case in general relativity). For further reading, the books of Besse (1987) and LeBrun and Wang (1999) are strongly recommended.

Basic Properties

Let (M, g) be a (pseudo)-Riemannian manifold. There is a unique connection ∇ , the Levi-Civita connection of g , with the following properties:

1. the torsion $T(X, Y) = \nabla_X Y - \nabla_Y X - [X, Y]$ vanishes and
2. $\nabla g = 0$

We can now form the Riemann curvature tensor of g :

$$R(X, Y)Z = \nabla_X \nabla_Y Z - \nabla_Y \nabla_X Z - \nabla_{[X, Y]} Z$$

This is a type (3,1) tensor. There is one nontrivial contraction we can perform to obtain a (2, 0) tensor, that is, the Ricci curvature

$$\text{Ric}(X, Y) = \text{tr}(Z \mapsto R(X, Z)Y)$$

We may perform a further contraction and obtain the scalar curvature $s = \text{tr}_g \text{Ric}$.

The Ricci curvature is a symmetric tensor of the same type as the metric, so we can make the following definition:

Definition 1 A metric g is Einstein if

$$\text{Ric} = \Lambda g \quad [1]$$

for some constant Λ .

In this article, we shall take g to be a Riemannian (positive-definite) metric.

Remark 1 In dimension higher than 2, we do not have to put in the assumption that Λ is constant by hand. For, taking the divergence of [1] gives $(1/2)ds = d\Lambda$, while taking instead the trace gives $s = n\Lambda$, so if $n \neq 2$, we see $d\Lambda = 0$.

Remark 2 In dimension 2 and 3, the Einstein condition is equivalent to constant curvature. The only complete Einstein manifolds in these dimensions are therefore the model spaces S^n, \mathbb{R}^n and

hyperbolic space, and quotients of these by discrete groups of isometries.

Remark 3 As noticed by Hilbert, the Einstein equations admit a variational interpretation. They are the variational equations for the total scalar curvature functional

$$g \mapsto \int_M s_g d\mu_g$$

restricted to the space of volume 1 metrics (here $d\mu_g$ denotes the volume form defined by g).

Obstructions

The most fundamental question, we can ask is:

Given a smooth manifold M does it support an Einstein metric?

One is also interested in the question of uniqueness of such a metric, or more generally of describing the moduli space of such metrics.

In this section we discuss obstructions to existence. In dimension 2 Remark 2 shows that any compact manifold admits an Einstein metric, while in dimension 3 the only possibilities are space forms. In particular, there is no Einstein metric on $S^1 \times S^2$.

The picture is much less clear in higher dimensions. If $\Lambda \geq 0$, one obtains some elementary obstructions just by considering the sign of the Ricci curvature:

1. If M supports a complete Einstein metric with $\Lambda > 0$, then by Myers's theorem M is compact and $\pi_1(M)$ is finite. Also there are obstructions coming from the positivity of the scalar curvature (e.g., if M is spin and $4m$ -dimensional, then the \hat{A} genus vanishes).
2. If M supports a complete Ricci-flat metric, then every finitely generated subgroup of $\pi_1(M)$ has polynomial growth.

However, if $\dim M \geq 5$, there is, at the time of writing, no known obstruction to M supporting an Einstein metric of negative Einstein constant.

In the borderline dimension 4, Hitchin and Thorpe observed that the Einstein condition put topological constraints on the manifold. For, we have the following expressions for the Euler characteristic χ and signature τ in terms of the curvature tensor:

$$\tau = \frac{1}{12\pi^2} \int_M |W_+|^2 - |W_-|^2 d\mu_g$$

$$\chi = \frac{1}{8\pi^2} \int_M |W_+|^2 + |W_-|^2 - |\text{Ric}_0|^2 + \frac{s^2}{24} d\mu_g$$

where W_+ and W_- are the self-dual and anti-self-dual parts of the Weyl tensor, s is the scalar curvature, and Ric_0 is the trace-free part of the Ricci tensor.

The Einstein condition is just $\text{Ric}_0 = 0$, so we immediately obtain the following inequality.

Theorem (Hitchin 1974). *A compact four-dimensional Einstein manifold satisfies the inequality*

$$|\tau| \leq \frac{2}{3}\chi$$

Note that equality is obtained if and only if g is Ricci-flat and (anti)-self-dual, which is equivalent to locally hyper-Kähler for some orientation. The only examples are the flat torus, the K3 surface with the Yau metric (now $\tau = 16$ and $\chi = 24$), and two quotients of K3.

Since the mid-1990s, LeBrun (2003) has obtained a series of results which sharpen the Hitchin–Thorpe inequality by obtaining estimates on the Weyl and scalar curvature terms. These estimates are obtained by using Seiberg–Witten theory, the general theme being that nonemptiness of the Seiberg–Witten moduli space gives lower bounds on the curvature terms. LeBrun shows there are infinitely many compact smooth simply connected 4-manifolds that satisfy the Hitchin–Thorpe inequality but nonetheless do not admit Einstein metrics.

Uniqueness and Moduli

In Yang–Mills theory, there is a highly developed theory of moduli spaces of instantons, including formulas for the dimension. The situation for Einstein metrics is far less well understood. The relevant moduli space here is the set of Einstein metrics modulo the action of the diffeomorphism group, but there are very few manifolds for which the moduli space has been determined. In dimension 2, of course, this is essentially the subject of the Teichmüller theory.

One example where the moduli space is understood is the K3 surface. As explained above, the Hitchin–Thorpe argument shows that any Einstein metric is hyper-Kähler, and the moduli space of such structures on K3 is understood as an open set in a certain noncompact symmetric space.

Some uniqueness results have been obtained in four dimensions. LeBrun used Seiberg–Witten techniques to show that the Einstein metric on a compact quotient of the complex hyperbolic plane $\mathbb{C}H^2$ is unique up to homotheties and diffeomorphisms. The analogous result for compact quotients of real hyperbolic 4-space was obtained using entropy methods by Besson, Courtois, and Gallot. It is still

unknown, however, whether nonstandard Einstein metrics can exist on S^4 .

In higher dimensions, very little is known. One can, by analogy with the theory of instantons, consider the linearization of the Einstein equations together with a further linear equation expressing orthogonality to the orbits of the diffeomorphism group. This gives a notion of formal tangent space to the Einstein moduli space. However, Koiso has shown that formal tangent vectors need not integrate to a curve of Einstein metrics. The structure of the moduli space (dimension, possible singularities) remains quite mysterious in general. It is known from the Wang–Ziller torus bundle examples that the moduli space can have infinitely many components.

Special Holonomy

Berger classified the possible holonomy groups of simply connected, irreducible, nonsymmetric n -dimensional Riemannian manifolds. The generic case is that of holonomy $\text{SO}(n)$, and there are six other possibilities, each of which corresponds to some special geometry. Interestingly, four of these are automatically Ricci-flat, while a fifth is Einstein with $\Lambda \neq 0$. The remaining example, that of Kähler geometry, is not automatically Einstein, but the Einstein equations with the additional Kähler assumption reduce to a scalar Monge–Ampère equation and are therefore simpler than the general Einstein system.

For further reading in this section, see the articles by Boyer–Galicki, Joyce, Salamon, Tian, Yau and the author in part I of LeBrun and Wang (1999), and also the book of Joyce (2000). For the Kähler case, see also Tian (2000).

Kähler Manifolds (Holonomy $\text{U}(n/2)$, $\text{SU}(n/2)$)

A Kähler manifold (M, g) admits a covariant constant complex structure I , and associated Kähler 2-form ω defined by $\omega(X, Y) = g(IX, Y)$. The Ricci form ρ is defined by $\rho(X, Y) = \text{Ric}(IX, Y)$, so the Einstein condition for a Kähler manifold becomes

$$\rho = \Lambda \omega$$

On a Kähler manifold, ρ is the curvature of the canonical bundle, so $[\rho/2\pi]$ is a representative for the cohomology class $c_1(M)$.

We see that a *necessary* condition for a complex manifold (M, I) to admit a Kähler–Einstein metric is that c_1 has a definite sign. We consider, in turn, the three cases:

$$c_1 < 0$$

In this case, we have:

Theorem (Aubin, Yau). *Let (M, I) be a compact complex manifold with $c_1 < 0$. Then (M, I) admits a Kähler–Einstein metric with $\Lambda < 0$. The metric is unique up to homothety.*

$$c_1 = 0$$

This is a special case of the Calabi conjecture, proved by Yau.

Theorem (Yau). *Let M be a compact Kähler manifold with Kähler form ω . For any closed real form ρ of type $(1, 1)$ with $[\rho/2\pi] = c_1(M)$, there exists a unique Kähler metric with Kähler form cohomologous to ω and Ricci form equal to ρ .*

In particular, if M is a compact Kähler manifold with $c_1 = 0$, there exists a Ricci-flat Kähler metric on M .

Ricci-flat Kähler metrics are called Calabi–Yau metrics, and are exactly the metrics with holonomy in $SU(n/2)$. They admit two parallel spinors and are of great interest to string theorists, because in some string theories spacetime is expected to be a product of the four-dimensional macroscopic factor with a compact Calabi–Yau manifold of complex dimension 3.

Yau’s theorem provides many examples of Calabi–Yau spaces. For example, we can take a nonsingular complex submanifold defined as a complete intersection by the vanishing of r polynomials of degree d_1, \dots, d_r in \mathbb{CP}^n . Now, M has complex dimension $n - r$ and $c_1 = 0$ if and only if $n + 1 = \sum_{i=1}^r d_i$. We obtain examples of complex dimension 2 by considering a quartic in \mathbb{CP}^3 , the intersection of a quadric and a cubic in \mathbb{CP}^4 , or the intersection of three quadrics in \mathbb{CP}^5 ; these all give examples of K3 surfaces. A famous example of a Calabi–Yau manifold of complex dimension 3 is given by the quintic in \mathbb{CP}^4 . This technique can be extended, for example, by considering complete intersections in weighted projective space or constructing Calabi–Yau desingularizations of singular spaces.

$$c_1 > 0$$

This case is the most complicated and, at the time of writing, is not yet fully understood. It is known that not every compact manifold with $c_1 > 0$ supports a Kähler–Einstein metric.

An early result of Matsushima was that the identity component of the automorphism group of a Kähler–Einstein space with $c_1 > 0$ must be reductive. This shows, for example, that the blow-up of \mathbb{CP}^2 at

one or two points does not admit a Kähler–Einstein metric, despite having $c_1 > 0$. (The one-point blow-up does admit a Hermitian–Einstein metric due to Page.) A second obstruction is the Futaki invariant, a character of the Lie algebra of the automorphism group. This character vanishes if there is a Kähler–Einstein metric.

Both the above obstructions depend on having a nontrivial algebra of holomorphic automorphisms of M . More recently, Tian has discovered further obstructions (in complex dimension 3 or higher) which can be present even if the automorphism algebra is trivial.

However, for compact complex surfaces with $c_1 > 0$, Tian has proved that vanishing of the Futaki invariant is sufficient. In particular, the blow-up of \mathbb{CP}^2 at k points in general position, where $3 \leq k \leq 8$, admits a Kähler–Einstein metric (note that $c_1^2 = 9 - k$ so if $k > 8$ then c_1 is no longer definite).

LeBrun–Catanese and Kotschick used these results to give an example of a topological 4-manifold carrying Einstein metrics of different signs. A deformation of the Barlow surface (a surface of general type) has $c_1 < 0$ and hence carries an Einstein metric with $\Lambda < 0$. But this space is homeomorphic (though not diffeomorphic) to the blow-up of \mathbb{CP}^2 at eight points, which carries an Einstein metric with $\Lambda > 0$. One may use this example to construct higher-dimensional examples of diffeomorphic manifolds carrying Einstein metrics of opposite sign.

Hyper-Kähler Manifolds (Holonomy $Sp(n/4)$)

These are always Ricci-flat. They have a triple (I, J, K) of covariant constant complex structures, satisfying the quaternionic multiplication relations $IJ = K = -JI$, etc., and defining Kähler forms $\omega_I, \omega_J, \omega_K$. Hyper-Kähler manifolds of dimension $n = 4N$ have $N + 1$ parallel spinors.

The most effective way of producing complete hyper-Kähler metrics has been the hyper-Kähler quotient construction (Hitchin *et al.* 1987), which was motivated by the Marsden–Weinstein quotient in symplectic geometry. Let G be a group acting freely on a hyper-Kähler manifold (M, g, I, J, K) preserving the hyper-Kähler structure. Subject to mild assumptions, we obtain a G -equivariant moment map $\mu: M \rightarrow \mathfrak{g}^* \otimes \mathbb{R}^3$, satisfying

$$d\mu_X(Y) = (\omega_I(X, Y), \omega_J(X, Y), \omega_K(X, Y))$$

Now the quotient $\mu^{-1}(0)/G$ is a hyper-Kähler manifold of dimension $\dim M - 4 \dim G$.

The power of this construction comes from the fact that even if M is just flat quaternionic space, one can obtain highly nontrivial quotients by suitable choice of group G (e.g., the asymptotically locally Euclidean four-dimensional examples of Kronheimer, which include as a subcase the multi-instanton metrics of Gibbons and Hawking).

Many examples of interest in mathematical physics may be obtained by taking hyper-Kähler quotients of an infinite-dimensional space of connections and Higgs fields (Hitchin 1987). Examples include moduli spaces of instantons over a hyper-Kähler base, moduli spaces of monopoles on \mathbb{R}^3 , and moduli spaces of Higgs pairs over a Riemann surface.

The hyper-Kähler manifolds produced so far by the quotient construction have all been noncompact. Examples of compact hyper-Kähler manifolds are rarer but some are known. Beauville has produced examples in all dimensions as desingularizations of symmetric products of the basic four-dimensional compact examples (K3 and the 4-torus).

Further material for this section may be found, for example, in Hitchin (1992) and in the chapter by the author on hyper-Kähler manifolds in LeBrun and Wang (1999).

Quaternionic Kähler Manifolds (Holonomy $\mathrm{Sp}(n/4)$ $\mathrm{Sp}(1)$)

These are always Einstein with nonzero Einstein constant. Instead of globally defined parallel complex structures as in the hyper-Kähler case, we have a sub-bundle \mathcal{G} of $\mathrm{End}(TM)$ with fiber isomorphic to the imaginary quaternions, parallel with respect to the Levi-Civita connection. Thus, we have locally defined almost-complex structures I, J, K , satisfying the quaternionic multiplication relations, such that covariant differentiation of one of I, J, K gives a linear combination of the other two. In particular, note that quaternionic Kähler manifolds are not Kähler.

If the Einstein constant Λ is positive, the only known complete examples are symmetric, the so-called compact Wolf spaces, which are in one-to-one correspondence with the compact simple Lie groups. It is conjectured that these are the only examples with $\Lambda > 0$, and some results in this direction have been established (e.g., it is known if $\dim M \leq 12$). It is also known that for fixed dimension, there are only finitely many types of compact quaternionic Kähler manifold with $\Lambda > 0$.

Many orbifold examples, however, are known to exist, for example, via the Galicki–Lawson quaternionic Kähler quotient construction.

If $\Lambda < 0$, more complete examples are known. In addition to the noncompact duals of the Wolf spaces, there are homogeneous, nonsymmetric examples due to Alekseevski, and infinite-dimensional families of inhomogeneous examples constructed via twistor methods by LeBrun (see also Biquard (2000)).

Exceptional Holonomy (G_2 or $\mathrm{Spin}(7)$)

Such metrics exist in dimension 7 or 8, respectively. They are always Ricci-flat and admit a parallel spinor. Local examples were constructed by Bryant using Cartan–Kähler theory, and some explicit complete noncompact examples were produced by Salamon and Bryant using a cohomogeneity-1 construction. More complicated explicit noncompact examples have recently been produced by several authors (see Cvetič *et al.* (2003) for a survey). Compact examples were produced using analytical methods by Joyce, and later by Kovalev. Joyce starts with a flat singular metric on quotients of the seven- or eight-dimensional torus and constructs an approximate solution to the special holonomy condition on a resolution of this singular space. Then an analytic argument is used to show that an exact nearby solution exists.

For further reading, consult Joyce (2000) as well as the article by Joyce in LeBrun and Wang (1999).

There are also some interesting examples of Einstein metrics which, although not of special holonomy themselves, are closely related to special holonomy geometries. In recent years, these have yielded many new examples of compact Einstein manifolds in the work of Boyer, Mann, Galicki, Kollar, Rees, Piccinni, and Nakamaye.

Einstein–Sasaki Structures

There are several different ways of defining these, but the simplest is to say that (M, g) is Einstein–Sasaki if the cone $(\mathbb{R} \times M, dt^2 + t^2g)$ is Ricci-flat Kähler. Also, an Einstein–Sasaki manifold has a circle action with quotient a Kähler–Einstein orbifold. Existence theorems for such orbifold metrics have led to many examples of Einstein–Sasaki metrics, including families on odd-dimensional spheres.

3-Sasakian Structures

Again, we can define these in terms of cones; (M, g) has a 3-Sasakian structure if the cone over it is hyper-Kähler. The basic example is S^{4n+3} with associated cone $\mathbb{H}^n - \{0\}$. A 3-Sasakian manifold is always Einstein with positive Einstein constant.

The hyper-Kähler quotient construction induces a 3-Sasakian quotient, and many examples of compact 3-Sasakian manifolds have been produced as 3-Sasakian quotients of S^{4n+3} . In particular, there are examples in dimension 7 with arbitrarily large second Betti number, showing that one cannot, in general, expect compactness/finiteness results for Einstein moduli spaces without further assumptions.

Homogeneous Examples

Another strategy to study the Einstein equations is to reduce the difficulty of the problem by imposing symmetries. More precisely, we consider Einstein manifolds (M, g) with an isometric action of a Lie group G . In general, the Einstein equations with this symmetry will now involve r independent variables where r is the dimension of the stratified space M/G . We call r the *cohomogeneity* of the manifold.

In this section, we consider the situation where (M, g) is *homogeneous*, that is, when the action of G is transitive so $r=0$. The Einstein equations now reduce to a system of *algebraic* equations.

We may now write $M=G/K$, where K is the stabilizer of a point of M . We choose an Ad_K -invariant vector space complement \mathfrak{p} to \mathfrak{k} in \mathfrak{g} , and identify \mathfrak{p} with the tangent space to G/K at the identity coset. The key point is that G -invariant metrics on $M=G/K$ may now be identified with Ad_K -invariant inner products on \mathfrak{p} , which may, in turn, be studied by looking at the decomposition of \mathfrak{p} into irreducible representations of K .

In the special case when G/K is isotropy irreducible (i.e., \mathfrak{p} is an irreducible representation of K), both the metric g and its Ricci tensor are proportional by Schur's lemma, and hence g is automatically Einstein. Isotropy-irreducible homogeneous spaces have been classified by Kramer, Manturov, Wolf, and Wang-Ziller.

In the general case, the Einstein equations become a system of polynomial equations. Determining whether this system has a real positive solution is, in general, a highly nontrivial problem. However, the situation of homogeneous metrics is one area in which the variational formulation of the Einstein equations has proved highly successful.

We are now considering the scalar curvature functional on the finite-dimensional space of unit G -invariant metrics on G/K . The behavior of the scalar curvature functional is related to the structure of the lattice of intermediate subalgebras between the Lie algebras of K and G .

An early result along these lines (Wang and Ziller 1986) is that if K is maximal in G (compact), then G/K admits a G -invariant Einstein metric. The idea

of the proof is to show that maximality of K forces the scalar curvature functional on the space of volume-1 homogeneous metrics to be both bounded above and proper, and therefore to have a maximum.

These ideas have been greatly extended by Böhm, Wang, and Ziller. Given a compact connected homogeneous space G/K , they define a graph whose vertices are $\text{Ad}(K)$ -invariant subalgebras strictly intermediate between \mathfrak{g} and \mathfrak{k} . The edges correspond to inclusions between subalgebras. A component of the graph is called *toral* if all subalgebras \mathfrak{h} in this component are such that the identity component of H/K is abelian. They now show that if the graph has at least two nontoral components, then G/K admits a G -invariant Einstein metric. The Einstein metrics in the theorem are produced by a mountain pass argument and may have co-index 1, contrasting with the maxima of the earlier theorem.

Further advances in this direction have recently been made by Böhm. He associates to G/K a simplicial complex, and shows that nonzero homology groups of the complex imply the existence of higher co-index Einstein metrics.

One can also study homogeneous noncompact Einstein spaces with $\Lambda < 0$. It is conjectured by Alekseevski that for all such examples K is a maximal compact subgroup of G . The reader is referred to Heber (1998) for further information on the noncompact case.

The above results give some powerful existence results for Einstein metrics. However, there are examples known of homogeneous spaces G/K which admit no G -invariant Einstein metric (Wang and Ziller 1986). One such example is $\text{SU}(4)/\text{SU}(2)$, where $\text{SU}(2)$ is a maximal subgroup of $\text{Sp}(2) \subset \text{SU}(4)$.

Techniques similar to those in the homogeneous case have been used to construct Einstein metrics on total spaces of certain bundles, via Riemannian submersions. Some highlights are Jensen's exotic Einstein metrics on $(4n+3)$ -dimensional spheres, and the Wang-Ziller metrics on total spaces of torus bundles over products of Kähler-Einstein manifolds. The latter construction gives examples of spaces admitting volume-1 Einstein metrics with infinitely many Einstein constants Λ .

Examples of Higher Cohomogeneity

One can also look for Einstein metrics of higher cohomogeneity. Most progress has been made in the cohomogeneity-1 case, that is, where the principal orbit G/K of the action has real codimension one in

M (see Eschenburg and Wang (2000) for background on such metrics). On the open dense set in M which is the union of the principal orbits, we may write the metric as

$$dt^2 + g_t$$

where g_t is a t -dependent homogeneous metric on G/K . The Einstein equations are now a system of ordinary differential equations in t .

One may also add a special orbit G/H at one or both ends of the interval over which t ranges. This will impose boundary conditions on the ODEs. For the manifold structure to extend smoothly over the special orbit, H/K must be a sphere. Notice that if $\Lambda > 0$, then to obtain a complete metric M must be compact, so we must add two special orbits. If $\Lambda \leq 0$ and the metric is irreducible, then a Bochner argument tells us that M is noncompact. In the Ricci-flat case, the Cheeger–Gromoll theorem tells us that to obtain a complete irreducible metric, we must have exactly one special orbit, so M is topologically the total space of a vector bundle over the special orbit. In fact, most of the known examples even with $\Lambda < 0$ have a special orbit too.

The system of ODEs we obtain is still highly nonlinear and difficult to analyze in general. However, there are certain situations in which the equations, or a subsystem, can be solved in closed form. If we take G/K to be a principal circle bundle over a Hermitian symmetric space, Bérard Bergery (1982) showed that the resulting Einstein equations are solvable. (His work was inspired by the earlier example of Page, which corresponds to the case when $G/K = U(2)/U(1)$, a circle bundle over \mathbb{CP}^1 .) In fact, Bérard Bergery's construction works in greater generality as we obtain the same equations if G/K is replaced by any Riemannian submersion with circle fibers over a positive Kähler–Einstein space. This illustrates a general principle that systems arising as cohomogeneity-1 Einstein equations also typically arise from certain bundle ansätze without homogeneity assumptions.

Wang and Wang generalized this construction to be the case when the hypersurface in M is a Riemannian submersion with circle fibers over a product of an arbitrary number of Kähler–Einstein factors. Other solvable Einstein systems have been studied by, for example, Wang and Dancer.

It may also be possible in certain situations to get existence results without an explicit solution. This observation underlies the important work of Böhm (1998). He constructs cohomogeneity-1 Einstein metrics on certain manifolds with dimension between 5 and 9, including all the spheres in this

range of dimensions. The equations are not now solved in closed form, but it is possible to get a qualitative understanding of the flow and to show that certain trajectories will give metrics on the desired compact manifolds.

Böhm has also shown, in an analogous result to the homogeneous case, that there are examples of manifolds with a cohomogeneity-1 G -action which do not support any G -invariant Einstein metric.

So far, not much is known about Einstein metrics of higher cohomogeneity. An exception is the situation of self-dual Einstein metrics in dimension 4, where the self-dual condition greatly simplifies the resulting equations. Calderbank, Pedersen, and Singer have achieved a good understanding of such metrics with T^2 symmetry, including construction of such metrics on Hirzebruch–Jung resolutions of cyclic quotient singularities.

Analytical Methods

So far there is no really general analytical method for proving existence of global Riemannian Einstein metrics (although, of course, such techniques do exist in more restrictive situations of special holonomy).

Although the Einstein equations admit a variational formulation, this has (except for homogeneous metrics) not yielded general existence results. Note that the Wang–Ziller torus bundle examples at the end of the section “Homogeneous examples” show that the Palais–Smale condition does not hold in full generality.

One early suggestion was to adopt a minimax procedure. In each conformal class $[g]$, one looks for a minimizer of the volume-normalized scalar curvature. Such a minimizer always exists. One then takes the supremum over all conformal classes. The resulting supremum of the functional is called the Yamabe invariant $Y(M)$ of the manifold M . If a maximizer g exists, and $Y(M) \leq 0$, then g is Einstein.

However, striking work of Petean shows that this procedure must fail to produce an Einstein metric in many cases. He proves that if $\dim M \geq 5$ and M is simply connected, then the Yamabe invariant is non-negative. So, for such an M , any Einstein metric produced will have $\Lambda \geq 0$, and we know that this puts constraints on the topology of M .

Another possible technique is to use the Hamilton Ricci flow. If this converges as $t \rightarrow \infty$, the limiting metric is Einstein. However, it seems hard in higher dimensions to get control over the flow. In particular, the Wang–Ziller example in the section “Homogeneous examples” of a homogeneous space with no invariant Einstein metric shows that the flow may fail to converge (the Hamilton flow preserves the property of G -invariance).

Graham–Lee and Biquard have used analytical methods to produce Einstein deformations of hyperbolic space (real, complex, quaternionic, or Cayley). The idea is to show that a sufficiently small deformation of the conformal infinity of hyperbolic space can be extended to a deformation of the hyperbolic metric.

Recently, Anderson has shown the existence of Einstein metrics with $\Lambda < 0$ on a large class of manifolds obtained by Dehn filling from hyperbolic manifolds with toral ends. The strategy is to glue on to the hyperbolic metric copies of a simple explicit asymptotically hyperbolic metric, and to show that the resulting metric can be perturbed to an exact solution of the Einstein equations.

See also: Einstein Equations: Exact Solutions; Einstein Equations: Initial Value Formulation; Hamiltonian Reduction of Einstein's Equations; Several Complex Variables: Compact Manifolds; Singularities of the Ricci Flow.

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Einstein–Cartan Theory

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Introduction

Notation

Standard notation and terminology of differential geometry and general relativity are used in this article. All considerations are local, so that the four-dimensional spacetime M is assumed to be a smooth manifold diffeomorphic to \mathbb{R}^4 . It is endowed with a metric tensor g of signature $(1,3)$ and a linear connection defining the covariant differentiation of tensor fields. Greek indices range from 0 to 3 and refer to spacetime. Given a field of frames (e_μ) on M , and the dual field of coframes (θ^μ) , one can write the metric tensor as $g = g_{\mu\nu}\theta^\mu\theta^\nu$, where $g_{\mu\nu} = g(e_\mu, e_\nu)$

and Einstein's summation convention is assumed to hold. Tensor indices are lowered with $g_{\mu\nu}$ and raised with its inverse $g^{\mu\nu}$. General-relativistic units are used, so that both Newton's constant of gravitation and the speed of light are 1. This implies $\hbar = l^2$, where $l \approx 10^{-33}$ cm is the Planck length. Both mass and energy are measured in centimeters.

Historical Remarks

The Einstein–Cartan theory (ECT) of gravity is a modification of general relativity theory (GRT), allowing spacetime to have torsion, in addition to curvature, and relating torsion to the density of intrinsic angular momentum. This modification was put forward in 1922 by Élie Cartan, before the discovery of spin. Cartan was influenced by the work of the Cosserat brothers (1909), who considered besides an (asymmetric) force stress tensor also a moments stress tensor in a suitably

generalized continuous medium. Work done in the 1950s by physicists (Kondo, Bilby, Kröner, and other authors) established the role played by torsion in the continuum theory of crystal dislocations. A recent review (Ruggiero and Tartaglia 2003) describes the links between ECT and the classical theory of defects in an elastic medium.

Cartan assumed the linear connection to be metric and derived, from a variational principle, a set of gravitational field equations. He required, without justification, that the covariant divergence of the energy–momentum tensor be zero; this led to an algebraic constraint equation, bilinear in curvature and torsion, severely restricting the geometry. This misguided observation has probably discouraged Cartan from pursuing his theory. It is now known that conservation laws in relativistic theories of gravitation follow from the Bianchi identities and, in the presence of torsion, the divergence of the energy–momentum tensor need not vanish. Torsion is implicit in the 1928 Einstein theory of gravitation with teleparallelism. For a long time, Cartan’s modified theory of gravity, presented in his rather abstruse notation, unfamiliar to physicists, did not attract any attention. In the late 1950s, the theory of gravitation with spin and torsion was independently rediscovered by Sciama and Kibble. The role of Cartan was recognized soon afterward and ECT became the subject of much research; see Hehl *et al.* (1976) for a review and an extensive bibliography. In the 1970s, it was recognized that ECT can be incorporated within supergravity. In fact, simple supergravity is equivalent to ECT with a massless, anticommuting Rarita–Schwinger field as the source. Choquet–Bruhat considered a generalization of ECT to higher dimensions and showed that the Cauchy problem for the coupled system of Einstein–Cartan and Dirac equations is well posed. Penrose (1982) has shown that torsion appears in a natural way when spinors are allowed to be rescaled by a complex conformal factor. ECT has been generalized by allowing nonmetric linear connections and additional currents, associated with dilation and shear, as sources of such a “metric-affine theory of gravity” (Hehl *et al.* 1995).

Physical Motivation

Recall that, in special relativity theory (SRT), the underlying Minkowski spacetime admits, as its group of automorphisms, the full Poincaré group, consisting of translations and Lorentz transformations. It follows from the first Noether theorem that classical, special-relativistic field equations, derived from a variational principle, give rise to

conservation laws of energy–momentum and angular momentum. Using Cartesian coordinates (x^μ), abbreviating $\partial\varphi/\partial x^\rho$ to $\varphi_{,\rho}$ and denoting by $t^{\mu\nu}$ and $s^{\mu\nu\rho} = -s^{\nu\mu\rho}$ the tensors of energy–momentum and of intrinsic angular momentum (spin), respectively, one can write the conservation laws in the form

$$t^{\mu\nu}_{;\nu} = 0 \quad [1]$$

and

$$(x^\mu t^{\nu\rho} - x^\nu t^{\mu\rho} + s^{\mu\nu\rho})_{,\rho} = 0 \quad [2]$$

In the presence of spin, the tensor $t^{\mu\nu}$ need not be symmetric,

$$t^{\mu\nu} - t^{\nu\mu} = s^{\mu\nu\rho}_{,\rho}$$

Belinfante and Rosenfeld have shown that the tensor

$$T^{\mu\nu} = t^{\mu\nu} + \frac{1}{2}(s^{\nu\mu\rho} + s^{\nu\rho\mu} + s^{\mu\rho\nu})_{,\rho}$$

is symmetric and its divergence vanishes.

In quantum theory, the irreducible, unitary representations of the Poincaré group correspond to elementary systems such as stable particles; these representations are labeled by the mass and spin.

In Einstein’s GRT, the spacetime M is curved; the Lorentz group – but not the Poincaré group – appears as the structure group acting on orthonormal frames in the tangent spaces of M . The energy–momentum tensor T appearing on the right-hand side of the Einstein equation is necessarily symmetric. In GRT there is no room for translations and the tensors t and s .

By introducing torsion and relating it to s , Cartan restored the role of the Poincaré group in relativistic gravity: this group acts on the affine frames in the tangent spaces of M . Curvature and torsion are the surface densities of Lorentz transformations and translations, respectively. In a space with torsion, the Ricci tensor need not be symmetric so that an asymmetric energy–momentum tensor can appear on the right-hand side of the Einstein equation.

Geometric Preliminaries

Tensor-Valued Differential Forms

It is convenient to follow Cartan in describing geometric objects as tensor-valued differential forms. To define them, consider a homomorphism $\sigma: \text{GL}_4(\mathbb{R}) \rightarrow \text{GL}_N(\mathbb{R})$ and an element $A = (A^\mu_\nu)$ of $\text{End } \mathbb{R}^4$, the Lie algebra of $\text{GL}_4(\mathbb{R})$. The derived representation of Lie algebras is given by

$$\frac{d}{dt} \sigma(\exp At)|_{t=0} = \sigma^\nu_\mu A^\mu_\nu$$

If (e_a) is a frame in \mathbb{R}^N , then $\sigma_\mu^\nu(e_a) = \sigma_{a\mu}^{b\nu} e_b$, where $a, b = 1, \dots, N$.

A map $a = (a^\mu_\nu): M \rightarrow \text{GL}_4(\mathbb{R})$ transforms fields of frames so that

$$e'_\mu = e_\nu a^\nu_\mu \quad \text{and} \quad \theta^\nu = a^\nu_\mu \theta'^\mu \quad [3]$$

A differential form φ on M , with values in \mathbb{R}^N , is said to be of type σ if, under changes of frames, it transforms so that $\varphi' = \sigma(a^{-1})\varphi$. For example, $\theta = (\theta^\mu)$ is a 1-form of type id. If now $A = (A^\mu_\nu): M \rightarrow \text{End } \mathbb{R}^4$, then one puts $a(t) = \exp tA: M \rightarrow \text{GL}_4(\mathbb{R})$ and defines the variations induced by an infinitesimal change of frames,

$$\begin{aligned} \delta\theta &= \frac{d}{dt} (a(t)^{-1}\theta)|_{t=0} = -A\theta \\ \delta\varphi &= \frac{d}{dt} (\sigma(a(t)^{-1})\varphi)|_{t=0} = -\sigma^\nu_\mu A^\mu_\nu \varphi \end{aligned} \quad [4]$$

Hodge Duals

Since M is diffeomorphic to \mathbb{R}^4 , one can choose an orientation on M and restrict the frames to agree with that orientation so that only transformations with values in $\text{GL}_4^+(\mathbb{R})$ are allowed. The metric then defines the Hodge dual of differential forms. Put $\theta_\mu = g_{\mu\nu}\theta^\nu$. The forms $\eta, \eta_\mu, \eta_{\mu\nu}, \eta_{\mu\nu\rho}$, and $\eta_{\mu\nu\rho\sigma}$ are defined to be the duals of $1, \theta_\mu, \theta_\mu \wedge \theta_\nu, \theta_\mu \wedge \theta_\nu \wedge \theta_\rho$, and $\theta_\mu \wedge \theta_\nu \wedge \theta_\rho \wedge \theta_\sigma$, respectively. The 4-form η is the volume element; for a holonomic coframe $\theta^\mu = dx^\mu$, it is given by $\sqrt{-\det(g_{\mu\nu})} dx^0 \wedge dx^1 \wedge dx^2 \wedge dx^3$. In SRT, in Cartesian coordinates, one can define the tensor-valued 3-forms

$$t^\mu = t^{\mu\nu}\eta_\nu \quad \text{and} \quad s^{\mu\nu} = s^{\mu\nu\rho}\eta_\rho \quad [5]$$

so that eqns [1] and [2] become

$$dt^\mu = 0 \quad \text{and} \quad dj^{\mu\nu} = 0$$

where

$$j^{\mu\nu} = x^\mu t^\nu - x^\nu t^\mu + s^{\mu\nu} \quad [6]$$

For an isolated system, the 3-forms t^μ and $j^{\mu\nu}$, integrated over the 3-space $x^0 = \text{const.}$, give the system's total energy-momentum vector and angular momentum bivector, respectively.

Linear Connection, Its Curvature and Torsion

A linear connection on M is represented, with respect to the field of frames, by the field of 1-forms

$$\omega^\mu_\nu = \Gamma^\mu_{\rho\nu} \theta^\rho$$

so that the covariant derivative of e_ν in the direction of e_μ is $\nabla_\mu e_\nu = \Gamma^\rho_{\mu\nu} e_\rho$. Under a change of frames [3], the connection forms transform as follows:

$$a^\mu_\rho \omega'^\rho_\nu = \omega^\mu_\rho a^\rho_\nu + da^\mu_\nu$$

If $\varphi = \varphi^a e_a$ is a k -form of type σ , then its covariant exterior derivative

$$D\varphi^a = d\varphi^a + \sigma^{a\mu}_{b\nu} \omega^\nu_\mu \wedge \varphi^b$$

is a $(k+1)$ -form of the same type. For a 0-form one has $D\varphi^a = \theta^\mu \nabla_\mu \varphi^a$. The infinitesimal change of ω , defined similarly as in [4], is $\delta\omega^\mu_\nu = DA^\mu_\nu$. The 2-form of curvature $\Omega = (\Omega^\mu_\nu)$, where

$$\Omega^\mu_\nu = d\omega^\mu_\nu + \omega^\mu_\rho \wedge \omega^\rho_\nu$$

is of type ad: it transforms with the adjoint representation of $\text{GL}_4(\mathbb{R})$ in $\text{End } \mathbb{R}^4$. The 2-form of torsion $\Theta = (\Theta^\mu)$, where

$$\Theta^\mu = d\theta^\mu + \omega^\mu_\nu \wedge \theta^\nu$$

is of type id. These forms satisfy the Bianchi identities

$$D\Omega^\mu_\nu = 0 \quad \text{and} \quad D\Theta^\mu = \Omega^\mu_\nu \wedge \theta^\nu$$

For a differential form φ of type σ , the following identity holds:

$$D^2\varphi^a = \sigma^{a\nu}_{b\mu} \Omega^\mu_\nu \wedge \varphi^b \quad [7]$$

The tensors of curvature and torsion are given by

$$\Omega^\mu_\nu = \frac{1}{2} R^\mu_{\nu\rho\sigma} \theta^\rho \wedge \theta^\sigma$$

and

$$\Theta^\mu = \frac{1}{2} Q^\mu_{\rho\sigma} \theta^\rho \wedge \theta^\sigma$$

respectively. With respect to a holonomic frame, $d\theta^\mu = 0$, one has

$$Q^\mu_{\rho\sigma} = \Gamma^\mu_{\sigma\rho} - \Gamma^\mu_{\rho\sigma}$$

In SRT, the Cartesian coordinates define a radius-vector field $X^\mu = -x^\mu$, pointing towards the origin of the coordinate system. The differential equation it satisfies generalizes to a manifold with a linear connection:

$$DX^\mu + \theta^\mu = 0 \quad [8]$$

By virtue of [7], the integrability condition of [8] is

$$\Omega^\mu_\nu X^\nu + \Theta^\mu = 0$$

Integration of [8] along a curve defines the Cartan displacement of X ; if this is done along a small closed circuit spanned by the bivector Δf , then the radius vector changes by about

$$\Delta X^\mu = \frac{1}{2} (R^\mu_{\nu\rho\sigma} X^\nu + Q^\mu_{\rho\sigma}) \Delta f^{\rho\sigma}$$

This holonomy theorem – rather imprecisely formulated here – shows that torsion bears to translations a relation similar to that of curvature to linear homogeneous transformations.

In a space with torsion, it matters whether one considers the potential of the electromagnetic field to be a scalar-valued 1-form φ or a covector-valued 0-form (φ_μ) . The first choice leads to a field $d\varphi$ that is invariant with respect to the gauge transformation $\varphi \mapsto \varphi + d\chi$. The second gives $\frac{1}{2}(\nabla_\mu \varphi_\nu - \nabla_\nu \varphi_\mu)\theta^\mu \wedge \theta^\nu = (D\varphi_\mu) \wedge \theta^\mu = d\varphi - \varphi_\mu \Theta^\mu$, a gauge-dependent field.

Metric-Affine Geometry

A metric-affine space (M, g, ω) is defined to have a metric and a linear connection that need not depend on each other. The metric alone determines the torsion-free Levi-Civita connection $\overset{\circ}{\omega}$ characterized by

$$d\theta^\mu + \overset{\circ}{\omega}_\nu^\mu \wedge \theta^\nu = 0 \quad \text{and} \quad \overset{\circ}{D}g_{\mu\nu} = 0$$

Its curvature is

$$\overset{\circ}{\Omega}_\nu^\mu = d\overset{\circ}{\omega}_\nu^\mu + \overset{\circ}{\omega}_\rho^\mu \wedge \overset{\circ}{\omega}_\nu^\rho$$

The 1-form of type ad,

$$\kappa^\mu{}_\nu = \omega^\mu{}_\nu - \overset{\circ}{\omega}_\nu^\mu \quad [9]$$

determines the torsion of ω and the covariant derivative of g ,

$$\Theta^\mu = \kappa^\mu{}_\nu \wedge \theta^\nu, \quad Dg_{\mu\nu} = -\kappa_{\mu\nu} - \kappa_{\nu\mu}$$

The curvature of ω can be written as

$$\Omega^\mu{}_\nu = \overset{\circ}{\Omega}_\nu^\mu + \overset{\circ}{D}\kappa^\mu{}_\nu \pm \kappa^\mu{}_\rho \wedge \kappa^\rho{}_\nu \quad [10]$$

The transposed connection $\tilde{\omega}$ is defined by

$$\tilde{\omega}_\nu^\mu = \omega_\nu^\mu + Q^\mu{}_{\nu\rho} \theta^\rho$$

so that, with respect to a holonomic frame, one has $\tilde{\Gamma}_{\nu\rho}^\mu = \Gamma_{\rho\nu}^\mu$. The torsion of $\tilde{\omega}$ is opposed to that of ω .

Riemann–Cartan Geometry

A Riemann–Cartan space is a metric-affine space with a connection that is metric,

$$Dg_{\mu\nu} = 0 \quad [11]$$

The metricity condition implies that $\kappa_{\mu\nu} + \kappa_{\nu\mu} = 0$ and $\Omega_{\mu\nu} + \Omega_{\nu\mu} = 0$. In a Riemann–Cartan space, the connection is determined by its torsion Q and the metric tensor. Let $Q_{\rho\mu\nu} = g_{\rho\sigma} Q^\sigma{}_{\mu\nu}$; then

$$\kappa_{\mu\nu} = \frac{1}{2}(Q_{\mu\sigma\nu} + Q_{\nu\mu\sigma} + Q_{\sigma\mu\nu})\theta^\sigma \quad [12]$$

The transposed connection of a Riemann–Cartan space is metric if and only if the tensor $Q_{\rho\mu\nu}$ is completely antisymmetric. Let $\tilde{\nabla}$ denote the

covariant derivative with respect to $\tilde{\omega}$. By definition, a symmetry of a Riemann–Cartan space is a diffeomorphism of M preserving both g and ω . The one-parameter group of local transformations of M , generated by the vector field ν , consists of symmetries of (M, g, ω) if and only if

$$\tilde{\nabla}^\mu \nu^\nu + \tilde{\nabla}^\nu \nu^\mu = 0 \quad [13]$$

and

$$D\tilde{\nabla}_\nu \nu^\mu + R^\mu{}_{\nu\rho\sigma} \nu^\rho \theta^\sigma = 0 \quad [14]$$

In a Riemannian space, the connections ω and $\tilde{\omega}$ coincide and [14] is a consequence of the Killing equation [13]. The metricity condition implies

$$D\eta_{\mu\nu\rho} = \eta_{\mu\nu\rho\sigma} \Theta^\sigma \quad [15]$$

The Einstein–Cartan Theory of Gravitation

An Identity Resulting from Local Invariance

Let (M, g, ω) be a metric-affine spacetime. Consider a Lagrangian L which is an invariant 4-form on M ; it depends on $g, \theta, \omega, \varphi$, and the first derivatives of $\varphi = \varphi^a e_a$. The general variation of the Lagrangian is

$$\delta L = L_a \wedge \delta\varphi^a + \frac{1}{2} \tau^{\mu\nu} \delta g_{\mu\nu} + \delta\theta^\mu \wedge t_\mu - \frac{1}{2} \delta\omega_\nu^\mu \wedge s^\nu{}_\mu + \text{an exact form} \quad [16]$$

so that $L_a = 0$ is the Euler–Lagrange equation for φ . If the changes of the functions g, θ, ω , and φ are induced by an infinitesimal change of the frames [4], then $\delta L = 0$ and [16] gives the identity

$$g_{\mu\rho} \tau^{\rho\nu} - \theta^\nu \wedge t_\mu + \frac{1}{2} Ds^\nu{}_\mu - \sigma_{a\mu}^{b\nu} L_a \wedge \varphi^b = 0$$

It follows from the identity that the two sets of Euler–Lagrange equations obtained by varying L with respect to the triples $(\varphi, \theta, \omega)$ and (φ, g, ω) are equivalent. In the sequel, the first triple is chosen to derive the field equations.

Projective Transformations and the Metricity Condition

Still under the assumption that (M, g, ω) is a metric-affine spacetime, consider the 4-form

$$8\pi K = \frac{1}{2} g^{\nu\rho} \eta_{\mu\rho} \wedge \Omega^\mu{}_\nu \quad [17]$$

which is equal to ηR , where $R = g^{\mu\nu} R_{\mu\nu}$ is the Ricci scalar; the Ricci tensor $R_{\mu\nu} = R^\rho{}_{\mu\rho\nu}$ is, in general, asymmetric. The form [17] is invariant with

respect to projective transformations of the connection,

$$\omega_\nu^\mu \mapsto \omega_\nu^\mu + \delta_\nu^\mu \lambda \quad [18]$$

where λ is an arbitrary 1-form. Projectively related connections have the same (unparametrized) geodesics. If the total Lagrangian for gravitation interacting with the matter field φ is $K + L$, then the field equations, obtained by varying it with respect to φ, θ , and ω are: $L_a = 0$,

$$\frac{1}{2} g^{\rho\sigma} \eta_{\mu\nu\rho} \wedge \Omega^\nu{}_\sigma = -8\pi t_\mu \quad [19]$$

and

$$D(g^{\mu\rho} \eta_{\rho\nu}) = 8\pi s^\mu{}_\nu \quad [20]$$

respectively. Put $s_{\mu\nu} = g_{\mu\rho} s^\rho{}_\nu$. If

$$s_{\mu\nu} + s_{\nu\mu} = 0 \quad [21]$$

then $s^\nu{}_\nu = 0$ and L is also invariant with respect to [18]. One shows that, if [21] holds, then, among the projectively related connections satisfying [20], there is precisely one that is metric. To implement properly the metricity condition in the variational principle, one can use the Palatini approach with constraints (Kopczyński 1975). Alternatively, following Hehl, one can use [9] and [12] to eliminate ω and obtain a Lagrangian depending on φ, θ , and the tensor of torsion.

The Sciama–Kibble Field Equations

From now on the metricity condition [11] is assumed, so that [21] holds and the Cartan field equation [20] is

$$\eta_{\mu\nu\rho} \wedge \Theta^\rho = 8\pi s_{\mu\nu} \quad [22]$$

Introducing the asymmetric energy–momentum tensor $t_{\mu\nu}$ and the spin density tensor $s_{\mu\nu\rho} = g_{\rho\sigma} s^\sigma{}_{\mu\nu}$ similarly as in [5], one can write the Einstein–Cartan equations [19] and [22] in the form given by Sciama and Kibble,

$$R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R = 8\pi t_{\mu\nu} \quad [23]$$

$$Q^\rho{}_{\mu\nu} + \delta_\mu^\rho Q^\sigma{}_{\nu\sigma} - \delta_\nu^\rho Q^\sigma{}_{\mu\sigma} = 8\pi s^\rho{}_{\mu\nu} \quad [24]$$

Equation [24] can be solved to give

$$Q^\rho{}_{\mu\nu} = 8\pi (s^\rho{}_{\mu\nu} + \frac{1}{2} \delta_\mu^\rho s^\sigma{}_{\nu\sigma} + \frac{1}{2} \delta_\nu^\rho s^\sigma{}_{\mu\sigma}) \quad [25]$$

Therefore, torsion vanishes in the absence of spin and then [23] is the classical Einstein field equation. In particular, there is no difference between the Einstein and Einstein–Cartan theories in empty space. Since practically all tests of relativistic gravity are based on consideration of

Einstein's equations in empty space, there is no difference, in this respect, between the Einstein and the Einstein–Cartan theories: the latter is as viable as the former.

In any case, the consideration of torsion amounts to a slight change of the energy–momentum tensor that can be also obtained by the introduction of a new term in the Lagrangian. This observation was made in 1950 by Weyl in the context of the Dirac equation.

In Einstein's theory, one can also satisfactorily describe spinning matter without introducing torsion (Bailey and Israel 1975).

Consequences of the Bianchi Identities: Conservation Laws

Computing the covariant exterior derivatives of both sides of the Einstein–Cartan equations, using [15] and the Bianchi identities, one obtains

$$8\pi D t_\mu = \frac{1}{2} \eta_{\mu\nu\rho\sigma} \Theta^\nu \wedge \Omega^{\rho\sigma} \quad [26]$$

and

$$8\pi D s_{\mu\nu} = \eta_{\nu\sigma} \wedge \Omega^\sigma{}_\mu - \eta_{\mu\sigma} \wedge \Omega^\sigma{}_\nu \quad [27]$$

Cartan required the right-hand side of [26] to vanish. If, instead, one uses the field equations [19] and [22] to evaluate the right-hand sides of [26] and [27], one obtains

$$D t_\mu = Q^\rho{}_{\mu\nu} \theta^\nu \wedge t_\rho - \frac{1}{2} R^\rho{}_{\sigma\mu\nu} \theta^\nu \wedge s^\sigma{}_\rho \quad [28]$$

and

$$D s_{\mu\nu} = \theta_\nu \wedge t_\mu - \theta_\mu \wedge t_\nu \quad [29]$$

Let v be a vector field generating a group of symmetries of the Riemann–Cartan space (M, g, ω) so that eqns [13] and [14] hold. Equations [28] and [29] then imply that the 3-form

$$j = v^\mu t_\mu + \frac{1}{2} \tilde{\nabla}^\nu v^\mu s_{\mu\nu}$$

is closed, $dj = 0$. In particular, in the limit of SRT, in Cartesian coordinates x^μ , to a constant vector field v there corresponds the projection, onto v , of the energy–momentum density. If $A^{\mu\nu}$ is a constant bivector, then $v^\mu = A^\mu{}_\nu x^\nu$ gives $j = j^{\mu\nu} A_{\mu\nu}$, where $j^{\mu\nu}$ is as in [6].

Spinning Fluid and the Generalized Mathisson–Papapetrou Equation of Motion

As in classical general relativity, the right-hand sides of the Einstein–Cartan equations need not necessarily be derived from a variational principle; they may be determined by phenomenological

considerations. For example, following Weyssenhoff, consider a spinning fluid characterized by

$$t^{\mu\nu} = P^\mu u^\nu \quad \text{and} \quad s^{\mu\nu\rho} = S^{\mu\nu} u^\rho$$

where $S^{\mu\nu} + S^{\nu\mu} = 0$ and u is the unit, timelike velocity field. Let $U = u^\mu \eta_\mu$ so that

$$t_\mu = P_\mu U \quad \text{and} \quad s_{\mu\nu} = S_{\mu\nu} U$$

Define the particle derivative of a tensor field φ^a in the direction of u by

$$\dot{\varphi}^a \eta = D(\varphi^a U)$$

For a scalar field φ , the equation $\dot{\varphi} = 0$ is equivalent to the conservation law $d(\varphi U) = 0$. Define $\rho = g_{\mu\nu} P^\mu u^\nu$, then [29] gives an equation of motion of spin

$$\dot{S}_{\mu\nu} = u_\nu P_\mu - u_\mu P_\nu$$

so that

$$P_\mu = \rho u_\mu + \dot{S}_{\mu\nu} u^\nu$$

From [28] one obtains the equation of translatory motion,

$$\dot{P}_\mu = (Q^\rho_{\mu\nu} P_\rho - \frac{1}{2} R^{\rho\sigma}_{\mu\nu} S_{\rho\sigma}) u^\nu$$

which is a generalization to the ECT of the Mathisson–Papapetrou equation for point particles with an intrinsic angular momentum.

From ECT to GRT: The Effective Energy–Momentum Tensor

Inside spinning matter, one can use [12] and [25] to eliminate torsion and replace the Sciama–Kibble system by a single Einstein equation with an effective energy–momentum tensor on the right-hand side. Using the split [10], one can write [23] as

$$\dot{R}_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R^\circ = 8\pi T_{\mu\nu}^{\text{eff}} \quad [30]$$

Here $\dot{R}_{\mu\nu}$ and \dot{R} are, respectively, the Ricci tensor and scalar formed from g . The term in [10] that is quadratic in κ contributes to T^{eff} an expression quadratic in the components of the tensor $s_{\mu\nu\rho}$, so that, neglecting indices, one can symbolically write

$$T^{\text{eff}} = T + s^2 \quad [31]$$

The symmetric tensor T is the sum of t and a term coming from $\dot{D}\kappa^\mu_\nu$ in [10]:

$$T^{\mu\nu} = t^{\mu\nu} + \frac{1}{2} \nabla^\rho (s^{\nu\mu\rho} + s^{\nu\rho\mu} + s^{\mu\rho\nu}) \quad [32]$$

It is remarkable that the Belinfante–Rosenfeld symmetrization of the canonical energy–momentum tensor appears as a natural consequence of ECT.

From the physical point of view, the second term on the right-hand side of [31], can be thought of as providing a spin–spin contact interaction, reminiscent of the one appearing in the Fermi theory of weak interactions.

It is clear from eqns [30]–[32] that whenever terms quadratic in spin can be neglected – in particular, in the linear approximation – ECT is equivalent to GRT. To obtain essentially new effects, the density of spin squared should be comparable to the density of mass. For example, to achieve this, a nucleon of mass m should be squeezed so that its radius r_{Cart} be such that

$$\left(\frac{l^2}{r_{\text{Cart}}^3} \right)^2 \approx \frac{m}{r_{\text{Cart}}^3}$$

Introducing the Compton wavelength $r_{\text{Compt}} = l^2/m \approx 10^{-13}$ cm, one can write

$$r_{\text{Cart}} \approx (l^2 r_{\text{Compt}})^{1/3}$$

The “Cartan radius” of the nucleon, $r_{\text{Cart}} \approx 10^{-26}$ cm, so small when compared to its physical radius under normal conditions, is much larger than the Planck length. Curiously enough, the energy l^2/r_{Cart} is of the order of the energy at which, according to some estimates, the grand unification of interactions is presumed to occur.

Cosmology with Spin and Torsion

In the presence of spinning matter, T^{eff} need not satisfy the positive-energy conditions, even if T does. Therefore, the classical singularity theorems of Penrose and Hawking can be overcome here. In ECT, there are simple cosmological solutions without singularities. The simplest such solution, found in 1973 by Kopczyński, is as follows. Consider a universe filled with a spinning dust such that $P^\mu = \rho u^\mu$, $u^\mu = \delta^\mu_0$, $S_{23} = \sigma$, and $S_{\mu\nu} = 0$ for $\mu + \nu \neq 5$, and both ρ and σ are functions of $t = x^0$ alone. These assumptions are compatible with the Robertson–Walker line element $dt^2 - \mathcal{R}(t)^2(dx^2 + dy^2 + dz^2)$, where $(x, y, z) = (x^1, x^2, x^3)$ and torsion is determined from [25]. The Einstein equation [23] reduces to the modified Friedmann equation,

$$\frac{1}{2} \dot{\mathcal{R}}^2 - M \mathcal{R}^{-1} + \frac{3}{2} S^2 \mathcal{R}^{-4} = 0 \quad [33]$$

supplemented by the conservation laws of mass and spin,

$$M = \frac{4}{3} \pi \rho \mathcal{R}^3 = \text{const.}, \quad S = \frac{4}{3} \pi \sigma \mathcal{R}^3 = \text{const.}$$

The last term on the left-hand side of [33] plays the role of a repulsive potential, effective at small values of \mathcal{R} ; it prevents the solution from vanishing. It should be

noted, however, that even a very small amount of shear in u results in a term counteracting the repulsive potential due to spin. Neglecting shear and making the (unrealistic) assumption that matter in the universe at $t=0$ consists of $\sim 10^{80}$ nucleons of mass m with aligned spins, one obtains the estimate $\mathcal{R}(0) \approx 1 \text{ cm}$ and a density of the order of m^2/l^4 , very large, but much smaller than the Planck density $1/l^2$.

Tafel (1975) found large classes of cosmological solutions with a spinning fluid, admitting a group of symmetries transitive on the hypersurfaces of constant time. The models corresponding to symmetries of Bianchi types I, VII₀, and V are nonsingular, provided that the influence of spin exceeds that of shear.

Summary

ECT is a viable theory of gravitation that differs very slightly from the Einstein theory; the effects of spin and torsion can be significant only at densities of matter that are very high, but nevertheless much smaller than the Planck density at which quantum gravitational effects are believed to dominate. It is possible that ECT will prove to be a better classical limit of a future quantum theory of gravitation than the theory without torsion.

See also: Cosmology: Mathematical Aspects; General Relativity: Overview.

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Einstein's Equations with Matter

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Introduction

Newton's theory of gravity with absolute time and Euclidean 3-space connects the gravitational potential U with its source, the density of matter ρ , by the Poisson equation

$$\Delta U = -4\pi\kappa\rho$$

where Δ is the Laplace operator and κ is the gravitational constant. The trajectories of massive test particles are the flow lines of the gradient of U .

Newton's theory has proven to be very accurate in the laboratory as well as in the solar system (except for a small discrepancy with the observed value of Mercury perihelion). Newton's theory together with special relativity, the equivalence principle, and ideas of Mach, have been an inspiration for Einstein to uncover the equations which must be satisfied by the geometry of spacetime. They link the curvature of the spacetime metric with a phenomenological symmetric 2-tensor T , which must represent the energy, momentum, and stresses of all the sources, by the equality:

$$S(g) \equiv \text{Ricci}(g) - \frac{1}{2}gR(g) = 8\pi\kappa T$$

where $\text{Ricci}(g)$ is the Ricci tensor of the spacetime metric g and $R(g)$ its scalar curvature. The symmetric 2-tensor $S(g)$ is called the Einstein tensor. The

Bianchi identities, due to the invariance of curvature by isometries of g , imply that the divergence of the Einstein tensor is identically zero: the Einstein equations imply therefore the vanishing of the divergence of the source tensor T . The equations so obtained generalize in a relativistic context the conservation laws of Newtonian mechanics. In local spacetime coordinates x^α , the Einstein equations and conservation laws read

$$S_{\alpha\beta} \equiv R_{\alpha\beta} - \frac{1}{2}g_{\alpha\beta}R = 8\pi\kappa T_{\alpha\beta}, \quad \nabla_\alpha T^{\alpha\beta} \equiv 0$$

where ∇ denotes the covariant derivative in the metric g .

The gravitational constant κ is inspired by the Newtonian equation relating the potential U with the density of matter. This equation can be obtained as an approximation of Einstein's equations with matter in the case of low velocities of matter and weak gravitational fields. The Newton's equation of motion of test particles is also an approximation of Einstein's geodesic motion of such particles which can be deduced from Einstein's equations themselves. However, if one wants to remain in the framework of the general relativity theory, it is these Einstein's equations which define the mass of a body, there is no comparison possible with some fixed given mass. As length had the dimension of time already in special relativity, now mass is found to have dimension of length. We write the equations in geometrical units, where $8\pi\kappa = 1$, keeping in mind the corresponding change to usual laboratory units only in specific applications. In geometrical units the mass of the Earth is of the order of the centimeter. The most precise measures of κ are still made using Newton type experiments, giving $\kappa = 6.67259 \times 10^{-11} \text{ m}^3 \text{ kg}^{-1} \text{ s}^{-2}$.

In the case of electromagnetic (or classical Yang-Mills) field sources, the stress energy tensor in special relativity is the well-known Maxwell tensor τ (or its generalizations), whose divergence vanishes when the field satisfies the Maxwell (or Yang-Mills) equations in vacuum. The expression of this tensor in a curved spacetime can be trivially deduced from its Minkowskian form. Its expression can also be deduced from the Lagrangian, and the vanishing of its divergence results from the invariance of this Lagrangian under isometries of the metric. It is the natural source of Einstein equations coupled with these fields. In the case of matter, the construction of a stress energy tensor is already delicate even in special relativity.

The simplest models of sources with well-understood properties – kinetic matter and perfect fluids – are reviewed in this article. Physical

situations difficult to model, even in special relativity, dissipative fluids and elasticity, are mentioned. The extension to electrically, or classical Yang-Mills-Higgs, charged matter, offers no conceptual difficulty, but interesting new situations.

Fluid Sources

A fluid source in a domain of a spacetime (V, g) is such that there exists, in this domain, a unit timelike vector field u , satisfying $g(u, u) \equiv g_{\alpha\beta}u^\alpha u^\beta = -1$, whose trajectories are the flow lines of matter. A moving Lorentzian orthonormal frame is called a proper frame if its timelike vector is u . Since the Einstein gravitational potentials reduce at a point in a Lorentzian orthonormal frame to Minkowskian values, one admits that the spacetime symmetric 2-tensor T , which embodies the density of stress, energy, and momentum of a given type of matter, in a proper frame takes the expression it would have in special relativity and inertial coordinates. The expression of T in a general frame results from its tensorial character and the equivalence principle. The problem is to find a good expression of T in special relativity.

Case of Dust (Incoherent Matter)

In a proper frame there is neither momentum nor stresses. Therefore, the stress energy tensor reads in a general frame, with r a scalar function representing the matter density:

$$T = ru \otimes u, \quad \text{i.e., } T_{\alpha\beta} = ru_\alpha u_\beta$$

Using the property $g(u, u) = -1$, the conservation laws imply the vanishing of the divergence of the matter flow ru , that is, the continuity equation (conservation of matter)

$$\nabla_\alpha (ru^\alpha) = 0$$

and the motion of the particles along geodesics of the metric:

$$u^\alpha \nabla_\alpha u^\beta = 0$$

Similar equations are obtained for a null dust model where $g(u, u) = 0$.

Perfect Fluid

Euler equations In Newtonian mechanics, a continuous matter flow is characterized by its mass density and flow velocity. The equations are a continuity equation (conservation of matter) and equations of motion resulting from Newton's law, which link the acceleration vector and the space

divergence of the stress symmetric 2-tensor whose contraction with the normal to a small 2-surface gives the force applied to it. A fluid is called perfect if the pressure it applies to a small surface element with normal n is independent of n . Its stress tensor t , symmetric 2-tensor on Euclidean space, is then invariant by rotations. By generalization, a relativistic fluid is called perfect if its stress energy tensor has the following form:

$$T_{\alpha\beta} = \mu u_\alpha u_\beta + p(g_{\alpha\beta} + u_\alpha u_\beta)$$

Then in a proper frame, where g takes the Minkowskian values and the only nonvanishing component of u is along the time axis and equal to 1, the projection of T on space is the Newtonian stress tensor with pressure p , while μ , the projection of T on the time axis, is the fluid energy density. There is no momentum density in the proper frame. The conservation laws, also called Euler equations, are shown to split, as in the case of dust, into a continuity equation

$$\nabla_\alpha[(\mu + p)u^\alpha] - u^\alpha \partial_\alpha p = 0$$

and equations of motion

$$(\mu + p)u^\alpha \nabla_\alpha u^\beta + (g^{\alpha\beta} + u^\alpha u^\beta) \partial_\alpha p = 0$$

In relativity, where mass and energy are equivalent, the continuity equation is no more a conservation law.

Equations of state As in Newtonian mechanics, the Euler equations must be completed by a relation, called equation of state, depending on the physical properties of the fluid. In general in addition to mechanics, thermodynamic properties must be considered. In relativity, they are borrowed from classical thermodynamics formulated in a spacetime context.

In the simplest cases one introduces a conserved rest mass density r (or particle number density for particles with rest mass zero), satisfying the equation

$$\nabla_\alpha P^\alpha = 0 \quad \text{with} \quad P^\alpha \equiv ru^\alpha$$

This r differs from the density of energy μ . One sets $\mu = r(1 + \varepsilon)$ and calls ε the internal specific energy. The first law of (reversible) thermodynamics is extended to relativistic perfect fluids by the identity

$$\Theta dS \equiv d\varepsilon + p d(r^{-1})$$

which defines both the absolute temperature Θ and the differential of the specific entropy S . Modulo the continuity equation and the thermodynamic identity, the matter conservation

is equivalent to the conservation of entropy along the flow lines:

$$\nabla_\alpha(rSu^\alpha) = 0 \quad \text{hence} \quad u^\alpha \partial_\alpha S = 0$$

The scalars p , μ , S , r are not independent. Simple situations can be modeled by an "equation of state" linking these quantities. In astrophysics, one is inspired by what is known from classical fluids, with additional relativistic considerations. General relativity plays a role in the case of strong gravitational field.

Very cold matter and nuclear matter are barotropic fluids; they obey an equation of state of the form $p = p(\mu)$.

When the energy μ is largely dominated by the radiation energy, the fluid is called ultrarelativistic. The Stefan-Boltzmann laws give $\mu = KT^4$ and $p = (1/3)KT^4$, hence $p = (1/3)\mu$; the stress energy tensor is traceless.

In white dwarves, the fluid is considered as polytropic: it obeys an equation of state of the form $p = f(S)r^\gamma$. If only the internal energy ε and pressure p are dominated by radiation, then $\varepsilon = Kr^{-1}T^4$ and $p = (1/3)KT^4$, hence $p = (1/3)r\varepsilon$. The use of the thermodynamic identity leads to $\gamma = 4/3$, $p = (K/3)(3S/4K)^{4/3}r^{4/3}$, with $\mu = 3p + r$.

For most other stars, the physical situation is too complex to be modeled by a simple equation; only tables of numerical values may be available.

In cosmology, there is little physical information about the fluid which is to represent the energy content of the universe. It is assumed that in the early universe of the big-bang models, at very high temperature, the fluid was ultrarelativistic. At later times, it is generally assumed, for simplicity, that there is an equation of state linear and independent of entropy, $p = (\gamma - 1)\mu$. In order that the speed of sound waves be not greater than the speed of light, one assumes that $1 \leq \gamma \leq 2$; $\gamma = 1$ corresponds to dust, $\gamma = 2$ to a stiff (see below) fluid.

Recent confrontations of theory and observations seem to imply the existence of a new, not directly seen, type of matter, called "dark matter."

Wave fronts and propagation speeds The wave fronts of a differential system are the submanifolds of spacetime whose normals n annul the characteristic determinant. Discontinuities propagate along wave fronts. For a hyperbolic system, the wave fronts determine the domain of dependence of a solution. For a perfect fluid, they are found to be

1. the matter wave fronts, generated by the flow lines, such that $u^\alpha n_\alpha = 0$ and

2. the sound wave fronts, whose normals satisfy the equation

$$D \equiv (p'_\mu - 1)(u^\alpha n_\alpha)^2 + p'_\mu n^\alpha n_\alpha = 0$$

in a proper frame at a point of spacetime $u^\alpha = \delta^\alpha_0$, $g_{\alpha\beta} = \eta_{\alpha\beta}$; this equation states that the slope of the spacetime normal to the wave front can be written as

$$\left(\frac{\sum (n_i)^2}{n_0^2} \right)^{1/2} = \frac{1}{\sqrt{p'_\mu}}$$

The sound propagation speed is the inverse of this slope, that is, $v = \sqrt{p'_\mu}$. It is less than the speed of light, as expected from a relativistic theory, if $p'_\mu \leq 1$. The limiting case where these speeds are equal is called incompressible or stiff fluid.

Hyperbolicity, existence, and uniqueness theorem The characteristics of the perfect fluid equations are real, but the apparent multiplicity of the matter wave fronts poses a problem for the hyperbolicity of the relativistic Euler equations, even in a given background metric. However, Choquet-Bruhat has proven that this system is a hyperbolic Leray system as well as its coupling with the Einstein equations, for instance, in wave gauge. The following theorem can then be proved using the general theorem on hyperbolic systems and an extension of the method used for Einstein's equations in vacuum.

Theorem *Let (M, \bar{g}, K) be an initial data set for the Einstein equations and $(\bar{u}, \bar{\mu}, \bar{S})$ be Cauchy data in a local Sobolev space H_s^{loc} , $s \geq 3$, on the 3-manifold M for a perfect fluid with a smooth equation of state. Suppose $\bar{\mu} > 0$ and $p'_\mu \leq 1$. There exists a globally hyperbolic spacetime of maximal extension solution of the Einstein equations with source such as perfect fluid taking these Cauchy data. Such a spacetime and fluid flow are smooth for smooth initial data. They are unique, up to spacetime isometries.*

The Euler equations have also been written as a first-order symmetric hyperbolic system by Bojllat, Ruggeri, and Strumia using general methods relying on the existence of a convex functional, and directly by Rendall, who pointed out the difficulty of modeling the general motion of isolated fluid bodies, because of the assumption $\bar{\mu} > 0$. He constructed some solutions without this assumption where the boundaries are freely falling. The general problem of determining the evolution of boundaries appears everywhere in general relativity, and in classical mechanics.

Global problems The spacetimes obtained above are, in general, incomplete: even in Minkowski spacetime, the Euler equations do not in general have solutions that are global in time. Shocks appear in relativistic perfect fluids as in classical ones. Global existence results have been obtained for four-dimensional ultrarelativistic fluids (limited data), and in the case of 1-space dimension. A detailed study of the global behavior of spherically symmetric solutions of the Einstein-Euler equations with equation of state admitting a phase transition from zero pressure to stiff fluid has been done by Christodoulou.

Dissipative Fluids

A general fluid stress energy tensor is with u , a unit vector whose trajectories are the flow lines:

$$T^{\alpha\beta} = \mu u^\alpha u^\beta + q^\alpha u^\beta + q^\beta u^\alpha + Q^{\alpha\beta}$$

with $q^\alpha u_\alpha = 0$, $Q^{\alpha\beta} u_\alpha = 0$

$\mu = T^{\alpha\beta} u_\alpha u_\beta$ is the energy density, which must satisfy $\mu \geq 0$, Q is a space tensor representing the stresses, orthogonal to u and q is a space vector considered as a heat flow. The fundamental equations are still $\nabla_\alpha T^{\alpha\beta} = 0$, but they must be implemented by constitutive equations for q and Q which do not have simple satisfactory answer in a relativistic context. The transfer of results from classical mechanics on viscous fluids or on heat transfer leads to propagation speeds greater than the speed of light. It should be remarked that these classical equations are obtained as governing asymptotic states; thus, the parabolic character of their relativistic version does not contradict relativistic causality. However, it would be interesting to obtain, for dissipative relativistic fluids, hyperbolic dissipative equations. Various systems have been proposed, in particular, by Marle by using an approximation near equilibrium of a solution of the relativistic Boltzmann equation. A promising system, also inspired from kinetic theory, is the "extended thermodynamics" of Müller and Ruggeri which takes as 14 fundamental unknowns, the vector $P = ru$ and the tensor T , satisfying the conservation laws. These equations are supplemented by equations linking a totally symmetric 3-tensor A with a symmetric 2-tensor I by equations of the form

$$\nabla_\alpha A^{\alpha\beta\gamma} = I^{\beta\gamma} \quad [1]$$

A and I are functions of P and T depending on the model and called constitutive equations. The system is shown to be symmetric hyperbolic under the existence of a convex entropy function, property which holds under appropriate physical assumptions.

Reasonable equations have been proposed and studied for several constituent fluids and superfluids.

Charged Fluids

The stress energy tensor of a charged fluid with electric (or Yang–Mills) charge is generally the sum of the stress energy tensor of the fluid and of the Maxwell (or Yang–Mills) field. This tensor is conserved modulo the Maxwell (or Yang–Mills) equations with source the electric current, and the Euler equations completed by the Lorentz force. The corresponding Einstein–Maxwell perfect fluid system is well posed in the case of zero or infinite conductivity (magnetohydrodynamics). A subtlety appears in the case of finite conductivity: the system is still well posed, but for a restricted (Gevrey) class of C^∞ fields.

Kinetic Models

Distribution Function and Moments

A general relativistic kinetic theory can be formulated without appeal to classical mechanics or special relativity. The matter is composed of particles whose size is negligible in the considered scale: rarefied gases in the laboratory, galaxies or even clusters of galaxies at the cosmological scale. The number of particles is so great and their motion so chaotic that the state of the matter can be described by a “one-particle distribution function,” a positive scalar function on the tangent bundle to the spacetime $(x, p) \mapsto f(x, p)$, which gives the mean number of particles with momentum p present at the point x of spacetime.

The first moment of f is a causal vector field P defined by the integral over the space \mathcal{P}_x of momenta at x , with ω_p a volume element in that space:

$$P(x) =: \int_{\mathcal{P}_x} p f(x, p) \omega_p$$

Out of the first moment, one extracts a scalar $r \geq 0$, interpreted as the square of a proper mass density given by $r^2 =: -g(P, P)$ and, if $r > 0$, a unit vector $u = r^{-1}P$ interpreted as the macroscopic flow velocity.

The second moment of the distribution function f is the symmetric 2-tensor on spacetime given by

$$T(x) =: \int_{\mathcal{P}_x} f(x, p) p \otimes p \omega_p$$

It is interpreted as the stress energy tensor of the distribution f . Higher moments are defined similarly.

Liouville–Vlasov Equation

When the gas is so rarefied that the particle trajectories do not cross, then in the absence of nongravitational forces, these trajectories are geodesics of g , orbits in TV of the vector field $X = (p^\alpha, Q^\alpha \equiv -\Gamma_{\lambda\mu}^\alpha p^\lambda p^\mu)$ with $\Gamma_{\lambda\mu}^\alpha$, the Christoffel symbols of g .

In a collisionless model, the physical law of conservation of particles imposes the conservation of f along the trajectories of X , that is, the Liouville–Vlasov equation

$$\mathcal{L}_X f \equiv p^\alpha \frac{\partial f}{\partial x^\alpha} + Q^\alpha \frac{\partial f}{\partial p^\alpha} = 0$$

Conservation laws If f satisfies the Vlasov equation, then all moments satisfy a conservation law, in particular,

$$\nabla_\alpha P^\alpha = 0 \text{ and } \nabla_\alpha T^{\alpha\beta} = 0$$

equations which make the Einstein–Vlasov system consistent.

The theory extends without problem to particles having the same rest mass m , because the scalar $g(p, p) = -m^2$ is constant on a geodesic.

Cauchy problem The Einstein–Vlasov system is an integro-differential system for g and f on a manifold $V = M \times R$. The Cauchy data for the spacetime metric g on $M_0 = M \times \{0\}$ is, as usual, a pair (\bar{g}, K) , implemented with gauge initial data which complete the definition of Cauchy data for a well-posed hyperbolic system in the chosen gauge. The Cauchy data for f are a function \bar{f} on the bundle P_{M_0} . It has been proved long ago that there exists a solution, geometrically unique, in a neighborhood of M_0 if the data are in Sobolev spaces, weighted by a power of p^0 in the case of \bar{f} .

Since the Vlasov matter model, solution of a linear equation for given g , has no singularity by itself, the Einstein–Vlasov system is a good candidate for solutions that are global in time. This global existence has been proved by Rein and Rendall in the case of small data, asymptotically flat with spherical symmetry or plane symmetry, or with hyperbolic symmetry and compact space. Global existence without these symmetries is an open problem.

Boltzmann Equation

When the particles undergo collisions, their trajectories in phase space are no more connected integral curves of the vector field X , that is, their moment

undergoes a jump with the crossing of another trajectory. In the Boltzmann model, the derivative $\mathcal{L}_X f$ is equal to the so-called collision operator, $\mathcal{I}f$:

$$(\mathcal{L}_X f)(x, p) = (\mathcal{I}f)(x, p)$$

where $\mathcal{I}f$ is an integral operator linked with the probability that two particles of momentum, respectively, p' and q' , collide at x and give, after the shock, two particles of momentum p and q . For "elastic" shocks, the total momentum is conserved, that is, p' and q' lie in the submanifold $\Sigma_{pq} = \{p' + q' = p + q\}$, with volume element ξ' and

$$(\mathcal{I}f)(x, p) \equiv \int_{\mathcal{P}_x} \int_{\Sigma_{pq}} [f(x, p')f(x, q') - f(x, p)f(x, q)] A(x, p, q, p', q') \xi' \wedge \omega_q$$

The function $A(x, p, q, p', q')$ is called the shock cross section; it is a phenomenological quantity. No explicit expression is known for it in relativity. A generally admitted property is the reversibility of elastic shocks, $A(x, p, q, p', q') = A(x, p', q', p, q)$. It can be proved that under this hypothesis, the first and second moment of f are conserved as in the collisionless case, making the Einstein–Boltzmann system consistent. Existence of solutions (that are local in time) of the Cauchy problem for this system has long been known. No global existence for the coupled system is known yet.

One defines, in a relativistic context, an entropy flux vector H which is proved to satisfy an H -theorem, that is, $\nabla_\alpha H^\alpha \geq 0$. In an expanding universe, for instance, Robertson Walker, where H depends only on time and an entropy density is defined by H^0 , one finds that a decrease in entropy is linked with the expansion of the universe, thus permitting its ever-increasing organization from an initial anisotropy of f in momentum space.

Other Matter Sources

Elastic Media

There are no solids in general relativity; in special relativity rigid motions are already very restricted. A theory of elastic deformations can only be defined relatively to some *a priori* given state of matter whose perturbations will satisfy laws analogous to the classical laws. Various such theories have been proposed through geometric considerations, extending methods of classical elasticity; they have been used to predict the possible signals from bar detectors of gravitational waves, or the motions in the crust of neutron stars. A general theory constructed by Lagrangian formalism has recently been developed.

Spinor Sources

A symmetric stress energy tensor can be associated to classical spinors of spin 1/2, leading to a well-posed Einstein–Dirac system. The theories of super-gravity couple the Einstein–Cartan equations with anticommuting spin 3/2 sources.

See also: Boltzmann Equation (Classical and Quantum); Einstein Equations: Exact Solutions; Einstein Equations: Initial Value Formulation; General Relativity: Overview; Geometric Analysis and General Relativity; Kinetic Equations; Spinors and Spin Coefficients.

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Electric-Magnetic Duality

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Introduction

Classical electromagnetism is described by Maxwell's equations, which, in 3-vector notation and corresponding respectively to the laws of Coulomb, Ampère, Gauss, and Faraday, are given by eqns [1a]–[1d]:

$$\operatorname{div} \mathbf{E} = \rho \quad [1a]$$

$$\operatorname{curl} \mathbf{B} - \frac{\partial \mathbf{E}}{\partial t} = \mathbf{J} \quad [1b]$$

$$\operatorname{div} \mathbf{B} = 0 \quad [1c]$$

$$\operatorname{curl} \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0 \quad [1d]$$

Equivalently, in covariant 4-vector notation, these correspond to eqns [2a] and [2b]:

$$\partial_\nu F^{\mu\nu} = -j^\mu \quad [2a]$$

$$\partial^*_\nu F^{\mu\nu} = 0 \quad [2b]$$

In eqns [1], \mathbf{E} and \mathbf{B} are the electric and magnetic fields, respectively, ρ is the electric charge density, and \mathbf{J} is the electric current. In eqns [2], $F_{\mu\nu}$ is the field tensor, $*F_{\mu\nu}$ the dual field tensor, and j^μ is the 4-current, related to the previous vector quantities by the following relations:

$$F_{\mu\nu} = \begin{pmatrix} 0 & E_1 & E_2 & E_3 \\ -E_1 & 0 & -B_3 & B_2 \\ -E_2 & B_3 & 0 & -B_1 \\ -E_3 & -B_2 & B_1 & 0 \end{pmatrix}$$

$$*F_{\mu\nu} = \begin{pmatrix} 0 & B_1 & B_2 & B_3 \\ -B_1 & 0 & E_3 & -E_2 \\ -B_2 & -E_3 & 0 & E_1 \\ -B_3 & E_2 & -E_1 & 0 \end{pmatrix}$$

$$j^\mu = (\rho, \mathbf{J})$$

Throughout this article, we shall denote the three spatial indices by lower-case Latin letters such as i, j , while Greek indices such as μ, ν denote spacetime indices running through 0, 1, 2, 3. The Einstein summation convention is used, whereby repeated indices are summed. Spacetime indices are raised

and lowered by the (flat) Minkowski metric $g_{\mu\nu} = \operatorname{diag}(1, -1, -1, -1)$. We also use units conventional in particle physics, in which the reduced Planck constant \hbar and the speed of light c are both set to 1.

In terms of the totally skew symmetric symbol $\varepsilon_{\mu\nu\rho\sigma}$ (with $\varepsilon_{0123} = 1$), the two field tensors are related by eqn [3]:

$$*F_{\mu\nu} = -\frac{1}{2}\varepsilon_{\mu\nu\rho\sigma}F^{\rho\sigma} \quad [3]$$

We say that $*F_{\mu\nu}$ is the dual of $F_{\mu\nu}$, and eqn [3] is indeed a duality relation because eqn [4] holds, which means that up to a sign, $F_{\mu\nu}$ and $*F_{\mu\nu}$ are duals of each other:

$$*(F) = -F \quad [4]$$

This duality is in fact the Hodge duality between p -forms and $(n-p)$ -forms in an n -dimensional space. In our particular case, $p=2$ and $n=4$, so that both F and its dual are 2-forms. The minus sign in eqn [4] comes about because of the Lorentzian (or pseudo-Riemannian) signature of Minkowski spacetime.

The physical significance of this duality is that such a symmetry interchanges electric and magnetic fields (again up to sign) (eqn [5]), as can be seen from the matrix representation of $F_{\mu\nu}$ and $*F_{\mu\nu}$ above:

$$*: \mathbf{E} \mapsto \mathbf{B}, \mathbf{B} \mapsto -\mathbf{E} \quad [5]$$

Now in the absence of electric charges and currents, one sees immediately that Maxwell's equations [1] or [2] are dual symmetric. This means that, *in vacuo*, whether we call an electromagnetic field electric or magnetic is a matter of convention. As far as the dynamics is concerned, there is no distinction.

On the other hand, eqns [1] and [2] as presented, that is, in the presence of matter, are manifestly not dual symmetric. The underlying reason for this asymmetry has been much studied both in physics and in mathematics. One of the two questions that this article addresses is precisely this. Following on this, we shall see what happens if we try somehow to restore this dual symmetry even in the presence of matter.

The second question that we wish to discuss is a generalization of this duality. Electromagnetism is a gauge theory, in which the gauge group is the abelian circle group $U(1)$, representing the phase of wave-functions in quantum mechanics. A physically relevant generalization, in which the abelian $U(1)$ is replaced by a nonabelian group (e.g., $SU(2)$, $SU(3)$)

is called Yang-Mills theory (Yang and Mills 1954), which is the theoretical basis of all modern particle physics. We shall show in this article how the concept of electric-magnetic duality can be generalized in the context of Yang-Mills theory.

Gauge Invariance, Sources, and Monopoles

Electric-magnetic duality, whether in the well-known abelian case or in the still somewhat open nonabelian case, is intimately connected with gauge invariance, sources, and monopoles, and also the dynamics as embodied in the gauge action. These questions in turn find their natural setting in differential geometry, particularly the geometry of fibre bundles.

Although classical electrodynamics can be fully described by the field tensor $F_{\mu\nu}$, one needs to introduce the electromagnetic (or gauge) potential A_μ if one considers quantum mechanics, as has been beautifully demonstrated by the Bohm-Aharonov experiment. The two quantities are related by eqn [6]:

$$F_{\mu\nu}(x) = \partial_\nu A_\mu(x) - \partial_\mu A_\nu(x) \quad [6]$$

The fact that the phase of a wave function $\psi(x)$ (e.g., of the electron) is not a measurable quantity (although relative phases of course are) implies that we are free to make the following transformation:

$$\psi(x) \mapsto e^{ie\Lambda(x)}\psi(x) \quad [7]$$

This in turn implies an unobservable transformation [8] on the gauge potential, where $\Lambda(x)$ is a real-valued function on spacetime:

$$A_\mu(x) \mapsto A_\mu(x) + \partial_\mu \Lambda(x) \quad [8]$$

This invariance is called gauge invariance. Since in this abelian case $F_{\mu\nu}$ is gauge invariant, so are the Maxwell equations, for which we shall take from now on the covariant form [2]. Inasmuch as the Maxwell equations dictate the dynamics of electromagnetism, gauge invariance is an intrinsic ingredient even in the classical theory.

In Yang-Mills theory, the $U(1)$ phase $e^{ie\Lambda(x)}$ is replaced by an element $S(x)$ of a nonabelian group G , so that eqns [7], [8], and [6] become, respectively, eqns [9], [10], and [11]:

$$\psi(x) \mapsto S(x)\psi(x) \quad [9]$$

$$A_\mu(x) \mapsto S(x)A_\mu(x)S^{-1}(x) - \left(\frac{i}{g}\right)\partial_\mu S(x)S^{-1}(x) \quad [10]$$

$$F_{\mu\nu}(x) = \partial_\nu A_\mu(x) - \partial_\mu A_\nu(x) + ig[A_\mu(x), A_\nu(x)] \quad [11]$$

Here the electric coupling e is replaced by a general gauge coupling g . The quantities A_μ and $F_{\mu\nu}$ now take values in the Lie algebra of the Lie group G and the bracket is the Lie bracket. The wave function $\psi(x)$ takes values in a vector space on which an appropriate representation of G acts. Notice that now the field tensor $F_{\mu\nu}$ is no longer invariant, but only covariant:

$$F_{\mu\nu}(x) \mapsto S(x)F_{\mu\nu}(x)S^{-1}(x) \quad [12]$$

Next we consider the charges of gauge theory. For the moment, we wish to distinguish between two types of charges: sources and monopoles. These are defined with respect to the gauge field, which in turn is derivable from the gauge potential.

Source charges are those charges that give rise to a nonvanishing divergence of the field. For example, the electric current j due to the presence of the electric charge e occurs on the right-hand side of the first Maxwell equation, and is given in the quantum case by eqn [13], where γ^μ is a Dirac gamma matrix, identifiable as a basis element of the Clifford algebra over spacetime:

$$j^\mu = e\bar{\psi}\gamma^\mu\psi \quad [13]$$

In the Yang-Mills case, the first Maxwell equation is replaced by the Yang-Mills equation

$$D_\nu F^{\mu\nu} = -j^\mu, \quad j^\mu = g\bar{\psi}\gamma^\mu\psi \quad [14]$$

We define the covariant derivative D as in

$$D_\mu F^{\mu\nu} = \partial_\mu F^{\mu\nu} - ig[A_\mu, F^{\mu\nu}] \quad [15]$$

Monopole charges, on the other hand, are topological obstructions specified geometrically by nontrivial G -bundles over every 2-sphere S^2 surrounding the charge. They are classified by elements of $\pi_1(G)$, the fundamental group of G . They are typified by the (abelian) magnetic monopole as first discussed by Dirac in 1931.

Let us go into a little more detail about the Dirac magnetic monopole. If the field tensor $F_{\mu\nu}$ does come from a gauge potential A_μ as in eqn [6], then simple algebra will tell us that this implies $\partial_\nu^* F^{\mu\nu} = 0$ as in eqn [2]. Hence, we conclude the following:

$$\exists \text{ monopole} \implies A_\mu \text{ cannot be well defined everywhere}$$

The result is actually stronger. Suppose there exists a magnetic monopole at a certain point in spacetime, and, without loss of generality, we shall consider a static monopole. If we surround this point by a (spatial) 2-sphere Σ , then the magnetic flux out of the sphere is given by

$$\iint_{\Sigma} \mathbf{B} \cdot d\boldsymbol{\sigma} = \iint_{\Sigma^N} \mathbf{B} \cdot d\boldsymbol{\sigma} + \iint_{\Sigma^S} \mathbf{B} \cdot d\boldsymbol{\sigma} \quad [16]$$

Here Σ^N and Σ^S are the northern and southern hemispheres overlapping on the equator S . By Stokes' theorem, since $F_{\mu\nu}$ has no components $F_{0i} = E_i$, we have

$$\iint_{\Sigma^N} \mathbf{B} \cdot d\boldsymbol{\sigma} = \oint_S \mathbf{A} \cdot d\mathbf{s} \quad [17a]$$

$$\iint_{\Sigma^S} \mathbf{B} \cdot d\boldsymbol{\sigma} = \oint_{-S} \mathbf{A} \cdot d\mathbf{s} \quad [17b]$$

In eqn [17b], $-S$ means the equator with the opposite orientation. Hence, $\oint_S + \oint_{-S} = 0$. But this contradicts the assumption that there exists a magnetic monopole at the center of the sphere. Hence, we see that if a monopole exists, then A_μ will have at least a string of singularities leading out of it. This is the famous Dirac string.

The more mathematically elegant way to describe this is that the principal bundle corresponding to electromagnetism with a magnetic monopole is nontrivial, so that the gauge potential A_μ has to be patched (i.e., related by transition functions in the overlap). Consider the example of a static monopole of magnetic charge \tilde{e} . For any (spatial) sphere S_r of radius r surrounding the monopole, we cover it with two patches N, S as follows:

$$(N): 0 \leq \theta < \pi, 0 \leq \phi \leq 2\pi$$

$$(S): 0 < \theta \leq \pi, 0 \leq \phi \leq 2\pi$$

In each patch we define the following:

$$A_1^{(N)} = \frac{\tilde{e}y}{4\pi r(r+z)}$$

$$A_2^{(N)} = -\frac{\tilde{e}x}{4\pi r(r+z)}$$

$$A_3^{(N)} = 0$$

$$A_1^{(S)} = -\frac{\tilde{e}y}{4\pi r(r-z)}$$

$$A_2^{(S)} = \frac{\tilde{e}x}{4\pi r(r-z)}$$

$$A_3^{(S)} = 0$$

In the overlap (containing the equator), $A^{(N)}$ and $A^{(S)}$ are related by a gauge transformation:

$$A_i^{(N)} - A_i^{(S)} = \partial_i \Lambda \quad [18]$$

$$\Lambda = \left(\frac{\tilde{e}}{2\pi} \right) \tan^{-1} \left(\frac{y}{x} \right) = \frac{\tilde{e}\phi}{2\pi}$$

Notice that $A_i^{(N)}$ has a line of singularity along the negative z -axis (which is the Dirac string

in this case); similarly for $A_i^{(S)}$ along the positive z -axis.

Furthermore, the corresponding field strength is given by

$$\mathbf{E} = 0 \quad [19a]$$

$$\mathbf{B} = \frac{\tilde{e}\mathbf{r}}{4\pi r^3} \quad [19b]$$

If we now evaluate the "magnetic flux" out of S_r , we have

$$\iint_{S_r} \mathbf{B} \cdot d\boldsymbol{\sigma} = \oint_{\text{Equator}} (A_\mu^{(N)} - A_\mu^{(S)}) dx^\mu = \tilde{e} \quad [20]$$

In other words, in the presence of a magnetic monopole, the second half of Maxwell's equations is modified according to eqn [21], with \tilde{j}^μ given by eqn [22].

$$\left. \begin{aligned} \operatorname{div} \mathbf{B} &= \tilde{\rho} \\ \operatorname{curl} \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} &= \tilde{\mathbf{J}} \end{aligned} \right\}, \quad \partial_\nu {}^*F^{\mu\nu} = -\tilde{j}^\mu \quad [21]$$

$$\tilde{j}^\mu = \tilde{e} \bar{\psi} \gamma^\mu \psi \quad [22]$$

Furthermore, the form of eqn [21] tells us that a monopole of the $F_{\mu\nu}$ field can also be considered as a source of the ${}^*F_{\mu\nu}$ field. The two descriptions are equivalent.

How are the charges e and \tilde{e} related? The gauge transformation $S = e^{ie\Lambda}$ relating $A_\mu^{(N)}$ and $A_\mu^{(S)}$ must be well defined; that is, if one goes round the equator once, $\phi = 0 \rightarrow 2\pi$, one should get the same S . This gives

$$e\tilde{e} = 2\pi n, \quad n \in \mathbb{Z} \quad [23]$$

In particular, the unit electric and magnetic charges are related by eqn [24], which is Dirac's quantization condition,

$$e\tilde{e} = 2\pi \quad [24]$$

So, in principle, just as in the electric case, where we could have charges $e, 2e, \dots$, here we could also have magnetic charges of $\tilde{e}, 2\tilde{e}, \dots$. In other words, both charges are quantized.

Another way to look at this is to consider the classification of principal bundles over S^2 . The reason for these topological 2-spheres is that we are interested in enclosing a point charge. For a nontrivial bundle, the patching is given by a function S defined in the overlap (the equator), in other words, a map $S^1 \rightarrow U(1)$. What this amounts to is a closed curve in the circle group $U(1)$. Now, curves that can be continuously deformed into one another cannot give

distinct fibre bundles, so that one sees easily that there exists a one-to-one correspondence:

$$\begin{array}{c} \{\text{principal } U(1) \text{ bundles over } S^2\} \\ \updownarrow \\ \{\text{homotopy classes of closed curves in } U(1)\} \end{array}$$

This last is $\pi_1(U(1)) \cong \mathbb{Z}$. Hence, we recover Dirac's quantization condition.

So, for electromagnetism, there are two equivalent ways of defining the magnetic charge, as a source or as a monopole:

1. $\partial_\nu {}^*F^{\mu\nu} = -\tilde{j}^\mu \propto n\tilde{e} \neq 0$.
2. An element of $\pi_1(U(1)) \cong \mathbb{Z}$.

The same goes for the electric charge. We also note that both definitions give us the fact that these charges are discrete (quantized) and conserved (invariant under continuous deformations).

We now want to apply similar considerations to the magnetic charges in the nonabelian case. For several (subtle) reasons the obvious expression $D_\nu {}^*F^{\mu\nu} \stackrel{?}{=} -\tilde{j}^\mu$ as a source (see Table 1) does not work. The quickest way to say this is that ${}^*F^{\mu\nu}$ in general has no corresponding potential \tilde{A}_μ and so is not a gauge field. Moreover, in contrast to the abelian case, the field tensor does not fully specify the physical field configuration, as demonstrated by Wu and Yang. We shall come back to this later.

But we have just seen that in the abelian case there is another equivalent definition, which is that a magnetic monopole is given by the gauge configuration corresponding to a nontrivial $U(1)$ bundle over S^2 . This can be generalized to the nonabelian case without any problem. Moreover, this definition automatically guarantees that a nonabelian monopole charge is quantized and conserved. This is the way monopoles are defined above.

Arguments similar to the abelian case easily yield the nonabelian analog of the Dirac quantization condition, eqn [25], the difference between the two cases being only a matter of conventional normalization.

$$g\tilde{g} = 4\pi \quad [25]$$

Table 1 Definitions of charges

	Sources	Monopoles
Abelian	$\partial_\nu F^{\mu\nu} = -j^\mu$	$\partial_\nu {}^*F^{\mu\nu} = -\tilde{j}^\mu$
Nonabelian	$D_\nu F^{\mu\nu} = -j^\mu$?

Abelian Duality and the Wu–Yang Criterion

We saw above the well-known fact that classical Maxwell theory is invariant under the duality operator. By this we mean that at any point in spacetime free of electric and magnetic charges we have the two dual symmetric Maxwell equations:

$$\partial_\nu {}^*F^{\mu\nu} = 0 \quad [dF = 0] \quad [26]$$

$$\partial_\nu F^{\mu\nu} = 0 \quad [d{}^*F = 0] \quad [27]$$

Displayed in square brackets are the equivalent equations in the language of differential forms. Then by the Poincaré lemma we deduce immediately the existence of potentials A and \tilde{A} such that eqns [28] and [29] hold:

$$F_{\mu\nu}(x) = \partial_\nu A_\mu(x) - \partial_\mu A_\nu(x) \quad [F = dA] \quad [28]$$

$${}^*F_{\mu\nu}(x) = \partial_\nu \tilde{A}_\mu(x) - \partial_\mu \tilde{A}_\nu(x) \quad [{}^*F = d\tilde{A}] \quad [29]$$

The two potentials transform independently under independent gauge transformations Λ and $\tilde{\Lambda}$:

$$A_\mu(x) \mapsto A_\mu(x) + \partial_\mu \Lambda(x) \quad [30]$$

$$\tilde{A}_\mu(x) \mapsto \tilde{A}_\mu(x) + \partial_\mu \tilde{\Lambda}(x) \quad [31]$$

This means that the full symmetry of this theory is doubled to $U(1) \times \tilde{U}(1)$, where the tilde on the second circle group indicates that it is the symmetry of the dual potential \tilde{A} . It is important to note that the physical degrees of freedom remain the same. This is clear because F and *F are related by an algebraic equation [3]. As a consequence, the physical theory is the same: the doubled gauge symmetry is there all the time but is just not so readily detected.

As mentioned in the Introduction, this dual symmetry means that what we call “electric” or “magnetic” is entirely a matter of choice.

In the presence of electric charges, the Maxwell equations usually appear as

$$\partial_\nu {}^*F^{\mu\nu} = 0 \quad [32]$$

$$\partial_\nu F^{\mu\nu} = -j^\mu \quad [33]$$

The apparent asymmetry in these equations comes from the experimental fact that there is only one type of charges observed in nature, which we choose to regard as a source of the field F (or, equivalently but unconventionally, as a monopole of the field *F). But as we see by dualizing eqns [32] and [33], that is, by interchanging the role of electricity and magnetism in relation to F , we could equally have thought of these instead as source charges of

the field *F (or, similarly to the above, as monopoles of F):

$$\partial_\nu {}^*F^{\mu\nu} = -\tilde{j}^\mu \quad [34]$$

$$\partial_\nu F^{\mu\nu} = 0 \quad [35]$$

If both electric and magnetic charges existed in nature, then we would have the dual symmetric pair:

$$\partial_\nu {}^*F^{\mu\nu} = -\tilde{j}^\mu \quad [36]$$

$$\partial_\nu F^{\mu\nu} = -j^\mu \quad [37]$$

This duality in fact goes much deeper, as can be seen if we use the Wu–Yang criterion to derive the Maxwell equations, although we should note that what we present here is not the textbook derivation of the Maxwell equations from an action, but we consider this method to be much more intrinsic and geometric. Consider first pure electromagnetism. The free Maxwell action is given by

$$\mathcal{A}_F^0 = -\frac{1}{4} \int F_{\mu\nu} F^{\mu\nu} \quad [38]$$

The true variables of the (quantum) theory are the A_μ , so in eqn [38] we should put in a constraint to say that $F_{\mu\nu}$ is the curl of A_μ [28]. This can be viewed as a topological constraint, because it is precisely equivalent to [26]. Using the method of Lagrange multipliers, we form the constrained action

$$\mathcal{A} = \mathcal{A}_F^0 + \int \lambda_\mu (\partial_\nu {}^*F^{\mu\nu}) \quad [39]$$

We can now vary this with respect to $F_{\mu\nu}$, obtaining eqn [40], which implies [27]:

$$F^{\mu\nu} = 2\varepsilon^{\mu\nu\rho\sigma} \partial_\rho \lambda_\sigma \quad [40]$$

Moreover, the Lagrange multiplier λ is exactly the dual potential \tilde{A} .

This derivation is entirely dual symmetric, since we can equally well use [27] as constraint for the action \mathcal{A}_F^0 , now considered as a functional of ${}^*F^{\mu\nu}$ (eqn [41]), and obtain [26] as the equation of motion:

$$\mathcal{A}_F^0 = \frac{1}{4} \int {}^*F_{\mu\nu} {}^*F^{\mu\nu} \quad [41]$$

This method applies to the interaction of charges and fields as well. In this case we start with the free field plus free particle action (eqn [42]), where we assume the free particle m to satisfy the Dirac equation,

$$\mathcal{A}^0 = \mathcal{A}_F^0 + \int \bar{\psi} (i\partial_\mu \gamma^\mu - m) \psi \quad [42]$$

To fix ideas, let us regard this particle carrying an electric charge e as a monopole of the potential \tilde{A}_μ . Then the constraint we put in is [33], giving

$$\mathcal{A}' = \mathcal{A}^0 + \int \tilde{\lambda}_\mu (\partial_\nu F^{\mu\nu} + j^\mu) \quad [43]$$

Variation with respect to *F gives eqn [32], and varying with respect to $\bar{\psi}$ gives

$$(i\partial_\mu \gamma^\mu - m)\psi = -eA_\mu \gamma^\mu \psi \quad [44]$$

So, the complete set of equations for a Dirac particle carrying an electric charge e in an electromagnetic field is [32], [33], and [44]. The duals of these equations will describe the dynamics of a Dirac magnetic monopole in an electromagnetic field.

We see from this that the Wu–Yang criterion actually gives us an intuitively clear picture of interactions. The assertion that there is a monopole at a certain spacetime point x means that the gauge field on a 2-sphere surrounding x has to have a certain topological configuration (e.g., giving a nontrivial bundle of a particular class), and if the monopole moves to another point then the gauge field will have to rearrange itself so as to maintain the same topological configuration around the new point. There is thus naturally a coupling between the gauge field and the position of the monopole, or, in physical language, a topologically induced interaction between the field and the charge (Wu and Yang, 1976). Furthermore, this treatment of interaction between field and matter is entirely dual symmetric.

As a side remark, consider that although the action \mathcal{A}_F^0 is not immediately identifiable as geometric in nature, the Wu–Yang criterion, by putting the topological constraint and the equation of motion on equal (or dual) footing, suggests that in fact it is geometric in a subtle manner not yet fully understood. Moreover, as pointed out, eqn [40] says that the dual potential is given by the Lagrange multiplier of the constrained action.

Nonabelian Duality Using Loop Variables

The next natural step is to generalize this duality to the nonabelian Yang–Mills case. Although there is no difficulty in defining ${}^*F^{\mu\nu}$, which is again given by [3], we immediately come to difficulties in the relation between field and potential; for example, as in eqn [11],

$$F_{\mu\nu}(x) = \partial_\nu A_\mu(x) - \partial_\mu A_\nu(x) + ig[A_\mu(x), A_\nu(x)]$$

First of all, despite appearances the Yang–Mills equation [45] (in the free-field case) and the Bianchi

identity [46] are not dual-symmetric, because the correct dual of the Yang–Mills equation ought to be given by eqn [47], where \tilde{D}_ν is the covariant derivative corresponding to a dual potential:

$$D_\nu F^{\mu\nu} = 0 \quad [45]$$

$$D_\nu {}^*F^{\mu\nu} = 0 \quad [46]$$

$$\tilde{D}_\nu {}^*F^{\mu\nu} = 0 \quad [47]$$

Secondly, the Yang–Mills equation, unlike its abelian counterpart [27], says nothing about whether the 2-form *F is closed or not. Nor is the relation [11] about exactness at all. In other words, the Yang–Mills equation does not guarantee the existence of a dual potential, in contrast to the Maxwell case. In fact, Gu and Yang have constructed a counterexample. Because the true variables of a gauge theory are the potentials and not the fields, this means that Yang–Mills theory is not symmetric under the Hodge star operation [3].

Nevertheless, electric–magnetic duality is a very useful physical concept, so one may wish to seek a more general duality transform ($\tilde{}$), satisfying the following properties:

1. $(\tilde{})^{\tilde{}} = \pm()$.
2. Electric field $F_{\mu\nu} \xleftrightarrow{\tilde{}} \text{magnetic field } \tilde{F}_{\mu\nu}$.
3. Both A_μ and \tilde{A}_μ exist as potentials (away from charges).
4. Magnetic charges are monopoles of A_μ , and electric charges are monopoles of \tilde{A}_μ .
5. $\tilde{}$ reduces to $*$ in the abelian case.

One way to do this is to study the Wu–Yang criterion more closely. This reveals the concept of charges as topological constraints to be crucial even in the pure field case, as can be seen in Figure 1. The point to stress is that, in the above abelian case, the condition for the absence of a topological charge (a monopole) exactly removes the redundancy of the variables $F_{\mu\nu}$, and hence recovers the potential A_μ .

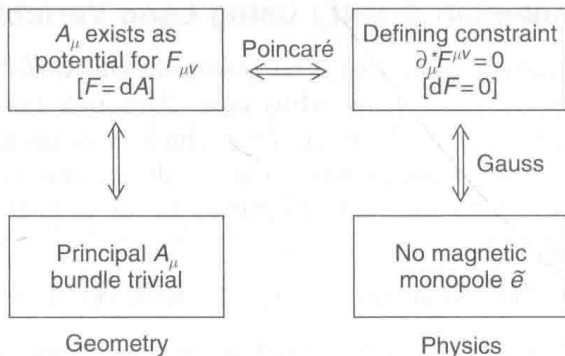


Figure 1

Now the nonabelian monopole charge was defined topologically as an element of $\pi_1(G)$, and this definition also holds in the abelian case of $U(1)$, with $\pi_1(U(1)) = \mathbb{Z}$. So the first task is to write down a condition for the absence of a nonabelian monopole.

To fix ideas, let us consider the group $SO(3)$, whose monopole charges are elements of \mathbb{Z}_2 , which can be denoted by a sign \pm . The vacuum, charge (+) (that is, no monopole) is represented by a closed curve in the group manifold of even winding number, and the monopole charge (−) by a closed curve of odd winding number. It is more convenient, however, to work in $SU(2)$, which is the double cover of $SO(3)$ and which has the topology of S^3 , as sometimes it is useful to identify the fundamental group of $SO(3)$ with the center of $SU(2)$ and hence consider the monopole charge as an element of this center. There the charge (+) is represented by a closed curve, and the charge (−) by a curve that winds an odd number of “half-times” round the sphere S^3 . Since these charges are defined by closed curves, it is reasonable to try to write the constraint in terms of loop variables. The treatment presented below is not as rigorous as some others, but the latter are not so well adapted to the problem in hand. Furthermore, it is important to emphasize that this approach aims to generalize electric–magnetic duality to Yang–Mills theory in direct and close analogy to duality in electromagnetism, without any further symmetries with which it may be expedient to enrich the theory. Other approaches are referred to in the next section.

Consider the gauge-invariant Dirac phase factor (or holonomy) $\Phi(C)$ of a loop C , which can be written symbolically as a path-ordered exponential:

$$\Phi[\xi] = P_s \exp i g \int_0^{2\pi} ds A_\mu(\xi(s)) \dot{\xi}^\mu(s) \quad [48]$$

In eqn [48], we parametrize the loop C as is eqn [49] and a dot denotes differentiation with respect to the parameter s .

$$C: \{ \xi^\mu(s) : s = 0 \rightarrow 2\pi, \xi(0) = \xi(2\pi) = \xi_0 \} \quad [49]$$

We thus regard loop variables in general as functionals of continuous piecewise smooth functions ξ of s . In this way, loop derivatives and loop integrals are just functional derivatives and functional integrals. This means that loop derivatives $\delta_\mu(s)$ are defined by a regularization procedure approximating delta functions with finite bump functions and then taking limits in a definite order. For functional integrals, there exist various regularization procedures, which are treated elsewhere in this Encyclopedia.

Polyakov (1980) introduces the logarithmic loop derivative of $\Phi[\xi]$:

$$F_\mu[\xi|s] = \frac{i}{g} \Phi^{-1}[\xi] \delta_\mu(s) \Phi[\xi] \quad [50]$$

This acts as a kind of “connection” in loop space since it tells us how the phase of $\Phi[\xi]$ changes from one loop to a neighbouring loop. One can go a step further and define its “curvature” in direct analogy with $F_{\mu\nu}(x)$ by

$$G_{\mu\nu}[\xi|s] = \delta_\nu(s) F_\mu[\xi|s] - \delta_\mu(s) F_\nu[\xi|s] + ig[F_\mu[\xi|s], F_\nu[\xi|s]] \quad [51]$$

It can be shown that by using the $F_\mu[\xi|s]$ we can rewrite the Yang–Mills action as eqn [52], where the normalization factor \bar{N} is an infinite constant:

$$\mathcal{A}_F^0 = -\frac{1}{4\pi\bar{N}} \int \delta\xi \int_0^{2\pi} ds \operatorname{tr}\{F_\mu[\xi|s] F^\mu[\xi|s]\} |\dot{\xi}(s)|^{-2} \quad [52]$$

However, the true variables of the theory are still the A_μ . They represent 4 functions of a real variable, whereas the loop connections represent 4 functionals of the real function $\xi(s)$. Just as in the case of the $F_{\mu\nu}$, these $F_\mu[\xi|s]$ have to be constrained so as to recover A_μ , but this time much more severely.

It turns out that, in pure Yang–Mills theory, the constraint that says there are no monopoles ([53]) also removes the redundancy of the loop variables, exactly as in the abelian case,

$$G_{\mu\nu}[\xi|s] = 0 \quad [53]$$

That this condition is necessary is easy to see by simple algebra. The proof of the converse of this “extended Poincaré lemma” is fairly lengthy. Granted this, we can now apply the Wu–Yang criterion to the action [52] and derive the Polyakov equation [54], which is the loop version of the Yang–Mills equation:

$$\delta_\mu(s) F^\mu[\xi|s] = 0 \quad [54]$$

In the presence of a monopole charge (–), the constraint [53] will have a nonzero right-hand side,

$$G_{\mu\nu}[\xi|s] = -J_{\mu\nu}[\xi|s] \quad [55]$$

The loop current $J_{\mu\nu}[\xi|s]$ can be written down explicitly. However, its global form is much easier to understand. Recall that $F^\mu[\xi|s]$ can be thought of as a loop connection, for which we can form its “holonomy.” This is defined for a closed (spatial) surface Σ (enclosing the monopole), parametrized by a family of closed curves $\xi_t(s)$, $t=0 \rightarrow 2\pi$. The “holonomy” Θ_Σ is then the total change in phase of $\Phi[\xi_t]$ as $t \rightarrow 2\pi$, and thus equals the charge (–).

To formulate an electric–magnetic duality that is applicable to nonabelian theory, one defines yet another set of loop variables. Instead of the Dirac phase factor $\Phi[\xi]$ for a complete curve [48], we consider the parallel phase transport for part of a curve from s_1 to s_2 :

$$\Phi_\xi(s_2, s_1) = P_s \exp ig \int_{s_1}^{s_2} ds A_\mu(\xi(s)) \dot{\xi}^\mu(s) \quad [56]$$

Then the new variables are defined by [57].

$$E_\mu[\xi|s] = \Phi_\xi(s, 0) F_\mu[\xi|s] \Phi_\xi^{-1}(s, 0) \quad [57]$$

These are not gauge invariant like $F_\mu[\xi|s]$ and may not be as useful in general, but seem more convenient for dealing with duality.

Using these variables, we now define their dual $\tilde{E}_\mu[\eta|t]$ according to

$$\begin{aligned} & \omega^{-1}(\eta(t)) \tilde{E}_\mu[\eta|t] \omega(\eta(t)) \\ &= -\frac{2}{\bar{N}} \varepsilon_{\mu\nu\rho\sigma} \dot{\eta}^\nu(t) \int \delta\xi ds E^\rho[\xi|s] \dot{\xi}^\sigma(s) \dot{\xi}^{-2}(s) \\ & \times \delta(\xi(s) - \eta(t)) \end{aligned} \quad [58]$$

In eqn [58], $\omega(x)$ is a (local) rotation matrix transforming from the frame in which the orientation in internal symmetry space of the fields $E_\mu[\xi|s]$ are measured to the frame in which the dual fields $\tilde{E}_\nu[\eta|t]$ are measured. It can be shown that this dual transform satisfies all five of the required conditions listed earlier.

Electric–magnetic duality in Yang–Mills theory is now fully reestablished using this generalized duality. We have the dual pairs of equations [59]–[60] and [61]–[62]:

$$\delta_\nu E_\mu - \delta_\mu E_\nu = 0 \quad [59]$$

$$\delta^\mu E_\mu = 0 \quad [60]$$

$$\delta^\mu \tilde{E}_\mu = 0 \quad [61]$$

$$\delta_\nu \tilde{E}_\mu - \delta_\mu \tilde{E}_\nu = 0 \quad [62]$$

Equation [59] guarantees that the potential A exists, and so is equivalent to [53], and hence is the nonabelian analog of [26]; while equation [60] is equivalent to the Polyakov version of Yang–Mills equation [54], and hence is the nonabelian analog of [27]. Equation [61] is equivalent by duality to [59] and is the dual Yang–Mills equation. Similarly equation [62] is equivalent to [60], and guarantees the existence of the dual potential \tilde{A} .

The treatment of charges using the Wu–Yang criterion also follows the abelian case, and will not be further elaborated here. For this and further details, the reader is referred to the original papers (Chan and Tsou 1993, 1999).

Also, just as in the abelian case, the gauge symmetry is doubled: from the group G we deduce that the full gauge symmetry is in fact $G \times \tilde{G}$, but that the physical degrees of freedom remain the same.

The above exposition establishes electric–magnetic duality in Yang–Mills theory only for classical fields. A hint that this duality persists at the quantum level comes from the work of 't Hooft (1978) on confinement. There he introduces two loop quantities $A(C)$ and $B(C)$ that are operators in the Hilbert space of quantum states satisfying the commutation relation [63] for an $SU(N)$ gauge theory, where n is the linking number between the two (spatial) loops C and C' :

$$A(C)B(C') = B(C')A(C) \exp(2\pi i n/N) \quad [63]$$

The order or Wilson operator is given explicitly by $A(C) = \text{tr } \Phi(C)$. These two operators play dual roles in the sense of electric–magnetic duality:

- $A(C)$ measures the magnetic flux through C and creates electric flux along C .
- $B(C)$ measures the electric flux through C and creates magnetic flux along C .

By defining the disorder operator $B(C)$ as the Wilson operator corresponding to the dual potential \tilde{A} obtained above, one can prove the commutation relation [63], thus showing that these classical fields, when promoted to operators, retain their duality relation. Furthermore, there is a remarkable relation between the two (abstractly identical) gauge groups, in that if one is confined then the dual must be broken (that is, in the Higgs phase). This result is known as 't Hooft's theorem.

The doubling of gauge symmetry, together with 't Hooft's theorem, has been applied to the confined colour group $SU(3)$ of quantum chromodynamics (QCD), in the Dualized Standard Model, to solve the puzzle of the existence of exactly three generations of fermions, with good observational support, by identifying the (necessarily broken) dual $SU(3)$ with the generation symmetry (Chan and Tsou, 2002).

Other Treatments of Nonabelian Duality

Since Yang–Mills theory is not symmetric under the Hodge $*$ -operation, there are several routes one can take to generalize the concept of electric–magnetic duality to the nonabelian case. What was presented in the last section is a modification of the $*$ -operation so as to restore this symmetry for Yang–Mills theory, keeping to the original gauge structure as much as possible. However, Yang–Mills theory as used today in particle and field theories are usually embedded in theories with more structures.

In the simplest case we have the Standard Model of Particle Physics, which describes all of particle interactions (except gravity) and which has the gauge group usually written as $SU(3) \times SU(2) \times U(1)$, corresponding to the $SU(3)$ of strong interaction and $SU(2) \times U(1)$ of electroweak interaction. [Strictly speaking, it is $(SU(3) \times SU(2) \times U(1))/\mathbb{Z}_6$, if we have the standard particle spectrum.] However, the former group is confined and the latter broken. The breaking is usually effected by introducing scalar fields called Higgs fields into the theory.

Besides the experimentally well-tested Standard Model, there are many theoretically popular models of gauge theory in which supersymmetry is postulated, thereby introducing extra symmetries into the theory. Many of these are remnants of string theory, and are usually envisaged as gauge theories in a spacetime dimension higher than 4.

Because of the extra structures and increased symmetries in these theories, there is quite a proliferation of concepts of duality, which could all be thought of as generalizations of abelian electric–magnetic duality (Schwarz, 1997). They come under the names of Seiberg–Witten duality, S-duality, T-duality, mirror symmetry, and so on. All these other aspects of duality have their own entries in this Encyclopedia.

See also: AdS/CFT Correspondence; Duality in Topological Quantum Field Theory; Four-Manifold Invariants and Physics; Large- N Dualities; Measure on Loop Spaces; Mirror Symmetry: a Geometric Survey; Nonperturbative and Topological Aspects of Gauge Theory; Seiberg–Witten theory; Standard Model of Particle Physics.

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Electroweak Theory

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Introduction

The discovery of the electroweak theory crowned long years of investigation on weak interactions. The key earlier developments included Fermi's phenomenological four-fermion interactions for the β -decay, discovery of parity violation and establishment of $V - A$ structure of the weak currents, the Feynman–Gell–Mann conserved vector current (CVC) hypothesis, current algebra and its beautiful applications in the 1960s, Cabibbo mixing and lepton–hadron universality, and finally, the proposal of intermediate vector bosons (IVBs) to mitigate the high-energy behavior of the pointlike Fermi's interaction theory.

It turned out that the scattering amplitudes in IVB theory still generally violated unitarity, due to the massive vector boson propagator,

$$\frac{-g^{\mu\nu} + q^\mu q^\nu / M^2}{q^2 - M^2 + i\epsilon}$$

The electroweak theory, known as Glashow–Weinberg–Salam (GWS) theory (Weinberg 1967, Salam 1968, Taylor 1976), was born through the attempts to make the hypothesis of IVBs for the weak interactions such that it is consistent with unitarity.

The GWS theory contains, and is in a sense a generalization of, quantum electrodynamics (QED) which was earlier successfully established as the quantum theory of electromagnetism in interaction with matter. GWS theory describes the weak and electromagnetic interactions in a single, unified gauge theory with gauge group

$$SU_L(2) \times U(1) \quad [1]$$

Part of this gauge symmetry is realized in the so-called “spontaneously broken” mode; only a $U_{EM}(1) \subset SU_L(2) \times U(1)$ subgroup, corresponding to the usual local gauge symmetry of the electromagnetism, remains manifest at low energies, with a massless gauge boson (photon). The other three gauge bosons W^\pm, Z , are massive, with masses ~ 80.4 and 91.2 GeV, respectively.

The theory is renormalizable, as conjectured by S Weinberg and by A Salam, and subsequently proved by G't Hooft (1971), and makes well-defined predictions order by order in perturbation theory.

Since the experimental observation of neutral currents (a characteristic feature of the Weinberg–Salam theory which predicts an extra, neutral massive vector boson, Z , as compared to the naive IVB hypothesis) at Gargamelle bubble chamber at CERN (1973), the theory has passed a large number of experimental tests. The first basic confirmation also included the discovery of various new particles required by the theory: the charm quark (SLAC, BNL, 1974), the bottom quark (Fermilab, 1977), and the tau (τ) lepton (SLAC, 1975). The heaviest top quark, having mass about two hundred times that of the proton, was found later (Fermilab, 1995). The direct observation of W and Z vector bosons was first made by UA1 and UA2 experiments at CERN (1983).

The GWS theory is today one of the most precise and successful theories in physics. Even more important, perhaps, together with quantum chromodynamics (QCD), which is a $SU(3)$ (color) gauge theory describing the strong interactions (which bind quarks into protons and neutrons, and the latter two into atomic nuclei), it describes correctly – within the present experimental and theoretical uncertainties – all the presently known fundamental forces in Nature, except gravity. The $SU(3)_{QCD} \times (SU_L(2) \times U(1))_{GWS}$ theory is known as the standard model (SM).

Both the electroweak (GSW) theory and QCD are gauge theories with a nonabelian (noncommutative) gauge group. This type of theories, known as Yang–Mills theories, can be constructed by generalizing the well-known gauge principle of QED to more general group transformations. It is a truly remarkable fact that all of the fundamental forces known today (apart from gravity) are described by Yang–Mills theories, and in this sense a very nontrivial unification can be said to underlie the basic laws of Nature (G't Hooft).

There are further deep and remarkable conditions (anomaly cancellations), satisfied by the structure of the theory and by the charges of experimentally known spin-1/2 elementary particles (see Tables 1 and 2), which guarantees the consistency of the theory as a quantum theory.

It should be mentioned, however, that the recent discovery of neutrino oscillations (SuperKamio-kande (1998), SNO, KamLAND, K2K experiments), which proved the neutrinos to possess nonvanishing masses, clearly indicates that the standard GWS theory must be extended, in an as yet unknown way.

Table 1 Quarks and their charges

Quarks	SU _L (2)	U _Y (1)	U _{EM} (1)
$\begin{pmatrix} u_L \\ d_L \end{pmatrix}, \begin{pmatrix} c_L \\ s_L \end{pmatrix}, \begin{pmatrix} t_L \\ b_L \end{pmatrix}$	$\underline{2}$	$\frac{1}{3}$	$\begin{pmatrix} \frac{2}{3} \\ -\frac{1}{3} \end{pmatrix}$
u_R, c_R, t_R	$\underline{1}$	$\frac{4}{3}$	$\frac{2}{3}$
d_R, s_R, b_R	$\underline{1}$	$-\frac{2}{3}$	$-\frac{1}{3}$

The primes indicate that the mass eigenstates are different from the states transforming as multiplets of SU_L(2) × U_Y(1). They are linearly related by CKM mixing matrix.

Table 2 Leptons and their charges

Leptons	SU _L (2)	U _Y (1)	U _{EM} (1)
$\begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix}, \begin{pmatrix} \nu_{\mu L} \\ \mu_L \end{pmatrix}, \begin{pmatrix} \nu_{\tau L} \\ \tau_L \end{pmatrix}$	$\underline{2}$	-1	$\begin{pmatrix} 0 \\ -1 \end{pmatrix}$
e_R, μ_R, τ_R	$\underline{1}$	-2	-1

The primes indicate again that the mass eigenstates are in different from the states transforming as multiplets of SU_L(2) × U_Y(1), as required by the observed neutrino oscillations.

The following is a brief summary of the GWS theory, its characteristic features, its implications to the symmetries of Nature, the status of the precision tests, and its possible extensions.

GWS Theory

All the presently known elementary particles (except for the gauge bosons W[±], Z, γ, the gluons, the graviton, possibly right-handed neutrinos) are listed in Tables 1–3 together with their charges with respect to the SU_L(2) × U(1) gauge group.

A doublet of Higgs scalar particles is included even though the physical component (which should appear as an ordinary scalar particle) has not yet been experimentally observed.

The Lagrangian is given by

$$\mathcal{L} = \mathcal{L}_{\text{gauge}} + \mathcal{L}_{\text{quarks}} + \mathcal{L}_{\text{leptons}} + \mathcal{L}_{\text{Higgs}} + \mathcal{L}_{\text{Yukawa}} + \mathcal{L}_{\text{g.f.}} + \mathcal{L}_{\text{ghosts}}$$

The gauge kinetic terms are

$$\mathcal{L}_{\text{gauge}} = -\frac{1}{4} \sum_{a=1}^3 F_{\mu\nu}^a F^{a\mu\nu} - \frac{1}{4} G_{\mu\nu} G^{\mu\nu}$$

Table 3 Higgs doublet scalars and their charges

Higgs doublet	SU _L (2)	U _Y (1)	U _{EM} (1)
$\begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix}$	$\underline{2}$	1	$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$

where

$$F_{\mu\nu}^a = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a + g\epsilon^{abc} A_\mu^b A_\nu^c$$
$$G_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu$$

are SU_L(2) × U(1) gauge field tensors; $\mathcal{L}_{\text{g.f.}}$ and \mathcal{L}_{FP} are the so-called gauge-fixing term and Faddeev–Popov ghost term, needed to define the gauge-boson propagators appropriately and to eliminate certain unphysical contributions. The gauge invariance of the theory is ensured by a set of identities (A Slavnov, J C Taylor). The quark kinetic terms have the form

$$\mathcal{L}_{\text{quarks}} = \sum_{\text{quarks}} \bar{\psi} i \gamma^\mu \mathcal{D}_\mu \psi$$

where \mathcal{D}_μ are appropriate covariant derivatives,

$$\mathcal{D}_\mu q_L = \left(\partial_\mu - \frac{ig}{2} \tau \cdot A_\mu - \frac{ig'}{6} B_\mu \right) q_L$$

for the left-handed quark doublets,

$$\mathcal{D}_\mu u_R = \left(\partial_\mu - \frac{2ig'}{3} B_\mu \right) u_R$$
$$\mathcal{D}_\mu d_R = \left(\partial_\mu + \frac{ig'}{3} B_\mu \right) d_R$$

and similarly for other “up” quarks c_R (charm) and t_R (top), and “down” quarks, s_R (strange), and b_R (bottom). Analogously, the lepton kinetic terms are given by

$$\mathcal{L}_{\text{leptons}} = \sum_{i=1}^3 \bar{\psi}^i i \gamma^\mu \mathcal{D}_\mu \psi^i$$
$$= \sum_{i=1}^3 \bar{\psi}_L^i i \gamma^\mu \left(\partial_\mu - ig \frac{\tau^a A_\mu^a}{2} + \frac{ig'}{2} B_\mu \right) \psi_L^i$$
$$+ \sum_{i=1}^3 \bar{\psi}_R^i i \gamma^\mu (\partial_\mu + ig' B_\mu) \psi_R^i$$

where ψ^i ($i = 1, 2, 3$) indicate the e, μ, τ lepton families; finally, the parts involving the Higgs fields are

$$\mathcal{L}_{\text{Higgs}} = \mathcal{D}_\mu \phi * \mathcal{D}^\mu \phi + V(\phi, \phi^\dagger)$$
$$V(\phi, \phi^\dagger) = -\mu^2 \phi^\dagger \phi - \lambda (\phi^\dagger \phi)^2$$

and

$$\mathcal{L}_{\text{Yukawa}} = \sum_{i,j=1}^3 \left[g_d^{ij} \bar{q}_L^i \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix} d_R^j + g_u^{ij} \bar{q}_L^i \begin{pmatrix} \phi^{0*} \\ -\phi^- \end{pmatrix} u_R^j \right] + \text{h.c.}$$
$$+ \sum_{i,j=1}^3 \left[g_e^i \bar{\psi}_L^i \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix} \psi_R^i \right] + \text{h.c.} \quad [2]$$

For $\mu^2 < 0$, the Higgs potential has a minimum at

$$\langle \phi^\dagger \phi \rangle = \langle |\phi^+|^2 + |\phi^0|^2 \rangle = -\frac{\mu^2}{2\lambda} \equiv \frac{v^2}{2} \neq 0$$

By choosing conveniently the direction of the Higgs field, its vacuum expectation value (VEV) is expressed as

$$\left\langle \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix} \right\rangle = \begin{pmatrix} 0 \\ v/\sqrt{2} \end{pmatrix}, \quad v \equiv \sqrt{-\frac{\mu^2}{\lambda}} \quad [3]$$

The physical properties of Higgs and gauge bosons are best seen by choosing the so-called unitary gauge,

$$\Phi(x) = \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix} = e^{i\zeta^a(x)\tau^a/v} \begin{pmatrix} 0 \\ (v + \eta(x))/\sqrt{2} \end{pmatrix} \equiv U(\zeta)\Phi'(x)$$

$$\psi_L = U(\zeta)\psi'_L, \quad \psi_R = \psi'_R$$

$$A_\mu = U(\zeta) \left(A'_\mu + \frac{i}{g} \partial_\mu \right) U^{-1}(\zeta), \quad A_\mu \equiv \frac{\tau^a A_\mu^a}{2}$$

and expressing everything in terms of primed variables. It is easy to see that

1. There is one physical scalar (Higgs) particle with mass,

$$m_\eta = \sqrt{-2\mu^2} \quad [4]$$

2. The Higgs kinetic term $(\mathcal{D}\phi^\dagger)(\mathcal{D}\phi')$ produces the gauge-boson masses

$$M_{W^\pm}^2 = \frac{g^2 v^2}{4}, \quad M_Z^2 = \frac{v^2}{4} (g^2 + g'^2) \quad [5]$$

3. The physical gauge bosons are the charged W^\pm , and two neutral vector bosons described by the fields

$$Z_\mu = \cos \theta_W A_{3\mu} - \sin \theta_W B_\mu,$$

$$A_\mu = \sin \theta_W A_{3\mu} + \cos \theta_W B_\mu$$

where the mixing angle

$$\theta_W = \tan^{-1} \frac{g'}{g} \quad \left(\sin \theta_W = \frac{g'}{\sqrt{g^2 + g'^2}} \right)$$

is known as the Weinberg angle. The massless A_μ field describes the photon.

Fermi Interactions and Neutral Currents

The fermions interact with gauge bosons through the charge and neutral currents

$$\mathcal{L} = \frac{g}{2} (J_{-\mu} W_+^\mu + J_{+\mu} W_-^\mu) + \mathcal{L}^{\text{n.c.}} \quad [6]$$

$$\mathcal{L}^{\text{n.c.}} = g J_\mu^3 A^{3\mu} + \frac{g'}{2} J_\mu^Y B^\mu$$

$$= e J_{\text{em}}^\mu A_\mu + \frac{g}{\cos \theta_W} J_\mu^0 Z^\mu \quad [7]$$

where

$$J_{+\mu} = \sum \bar{\psi}_L \gamma_\mu \tau^+ \psi_L$$

$$= \frac{1}{2} \sum \bar{\psi} \gamma_\mu \tau^+ (1 - \gamma_5) \psi$$

$$\equiv \frac{1}{2} J_{+\mu}^{V-A} \quad [8]$$

corresponds to the standard charged current, and

$$J_\mu^0 = J_\mu^3 - \sin^2 \theta_W J_\mu^{\text{em}} \quad [9]$$

is the neutral current to which the Z boson is coupled ($J_\mu^3 = (1/2) \sum \bar{\psi}_L \gamma_\mu \tau^3 \psi_L$ and J_μ^{em} is the electromagnetic current). The model thus predicts the existence of neutral current processes, mediated by the Z boson, such as $\nu_\mu e \rightarrow \nu_\mu e$ or $\bar{\nu}_\mu e \rightarrow \bar{\nu}_\mu e$, with cross section of the same order of that for the charged current process, $\bar{\nu}_e e \rightarrow \bar{\nu}_e e$, but with a characteristic L-R asymmetric couplings depending on the Weinberg angle. By eqn [9] appropriate ratios of cross sections, such as $\sigma(\nu_\mu e \rightarrow \nu_\mu e) / \sigma(\bar{\nu}_\mu e \rightarrow \bar{\nu}_\mu e)$, can be used to measure $\sin^2 \theta_W$.

The exchange of heavy W bosons generates an effective current-current interaction at low energies:

$$\mathcal{L}_{\text{eff}}^{\text{c.c.}} = -\frac{g^2}{2M_W^2} J_{-\mu} J_+^\mu$$

the well-known Fermi-Feynman-Gell-Mann Lagrangian $-\frac{G_F}{\sqrt{2}} J_{V-A}^\dagger J_{V-A}^\mu$, with

$$\frac{G_F}{\sqrt{2}} = \frac{g^2}{8M_W^2}$$

This means that the Higgs VEV must be taken to be

$$v = 2^{-1/4} G_F^{-1/2} \simeq 246 \text{ GeV} \quad [10]$$

Masses

It is remarkable that “all” known masses of the elementary particles – except perhaps those of the neutrino masses – are generated in GWS theory through the spontaneous breakdown of $SU_L(2) \times U(1)$ symmetry, through the Higgs VEV (eqns [3] and [10]). The boson masses are given by [4] and [5]. Note that the relation

$$\rho = \frac{M_W^2}{M_Z^2 \cos^2 \theta_W} = 1 + O(\alpha)$$

reflects an accidental $SO(3)$ symmetry present (note the $SO(4)$ symmetry of the Higgs potential in the limit $\alpha \rightarrow 0$, before the spontaneous breaking) in the model, called custodial symmetry. This is a characteristic, model-dependent feature of the minimal model, not

necessarily required by the gauge symmetry. This relation is well met experimentally, although a quantitative discussion requires the choice of the renormalization scheme (including the definition of $\sin \theta_W$ itself) and check of consistency with various other data.

The fermions get mass through the Yukawa interactions (eqn [2]); the fermion masses are arbitrary parameters of the model and cannot be predicted within the GWS theory. An important feature of this mechanism is that the coupling of the physical Higgs particle to each fermion is proportional to the mass of the latter. This should give a clear, unambiguous experimental signature for the Higgs scalar of the minimal GWS model.

The recent discovery of nonvanishing neutrino masses requires the theory to be extended. Actually, there is a natural way to incorporate such masses in the standard GWS model, by a minimal extension. As the right-handed neutrinos, if they exist, are entirely neutral with respect to the $SU_L(2) \times U(1)$ gauge symmetry, they do not need its breaking to have mass. In other words, ν_R may get Majorana masses, $\sim M_R \nu_R \nu_R$, by some yet unknown mechanism, much larger than those of other fermions (such a mechanism is quite naturally present in some grand unified models). If now the Yukawa couplings are introduced as for the quarks and for the down leptons, then the Dirac mass terms result upon condensation of the Higgs field, and the neutrino mass matrix would take the form, for one flavor (in the space of $(\nu_L, \bar{\nu}_R)$):

$$\begin{pmatrix} 0 & m_D \\ m_D & M_R \end{pmatrix} \quad [11]$$

Table 4 Quark masses

u (MeV)	c (GeV)	t (GeV)	d (MeV)	s (MeV)	b (GeV)
1.5–4	1.15–1.35	174.3 ± 5.1	4–8	80–130	4.1–4.4

Table 5 Leptons masses

ν_e (eV)	ν_μ (MeV)	ν_τ (MeV)
<3	<0.19	<18.2
e (MeV)	μ (MeV)	τ (MeV)
$0.51099892 \pm 4 \times 10^{-8}$	$105.658369 \pm 9 \times 10^{-6}$	1776.99 ± 0.26

Table 6 Gauge-boson masses

Photon	Gluons	W^\pm (GeV)	Z (GeV)
0	0	80.425 ± 0.038	91.1876 ± 0.0021

If the Dirac masses are assumed to be of the same order of those of the quarks and if the right-handed Majorana masses M_R are far larger, for example, of the order of the grand unified scale, $O(10^{16} \text{ GeV})$, then diagonalization of the mass matrix would give, for the physical masses of the left-handed neutrinos, $\sim m_D^2/M_R \ll m_D$, much smaller than other fermion masses, quite naturally (“see-saw” mechanism).

CKM Quark Mixing As there is *a priori* no reason why the weak-interaction eigenstates should be equal to the mass eigenstates, the Yukawa couplings in eqn [2] are in general nondiagonal matrices in the flavor. Suppose that the weak base for the quarks is given in terms of the mass eigenstates (in which quark masses are made diagonal), by unitary transformations

$$u_{Li} = \sum_j V_{ij}^{\text{up}} \tilde{u}_{Lj}, \quad d_{Li} = \sum_j V_{ij}^{\text{down}} \tilde{d}_{Lj}$$

then the interaction terms with W^\pm bosons [6] can be cast in the form (Kobayashi and Maskawa 1972)

$$\begin{aligned} \mathcal{L}^{\text{W-exc}} = & \bar{u}_L^i \gamma^\mu W_\mu^+ U_{ij}^{(\text{CKM})} d_L^j \\ & + \bar{d}_L^k \gamma^\mu W_\mu^- U_{k\ell}^{(\text{CKM})\dagger} u_L^\ell \end{aligned} \quad [12]$$

where $U_{ij}^{\text{CKM}} \equiv (V^{\text{up}\dagger} \cdot V^{\text{down}})_{ij}$ is called Cabibbo–Kobayashi–Maskawa (CKM) matrix. It can be parametrized in terms of three Euler angles and one phase

$$\begin{aligned} U = & \begin{pmatrix} U_{ud} & U_{us} & U_{ub} \\ U_{cd} & U_{cs} & U_{cb} \\ U_{td} & U_{ts} & U_{tb} \end{pmatrix} \\ = & \begin{pmatrix} c_{12}c_{13} & s_{12}c_{13} & s_{13}e^{-i\delta_{13}} \\ -s_{12}c_{23} - c_{12}s_{23}s_{13}e^{i\delta_{13}} & c_{12}c_{23} - s_{12}s_{23}s_{13}e^{i\delta_{13}} & s_{23}c_{13} \\ s_{12}s_{23} - c_{12}c_{23}s_{13}e^{i\delta_{13}} & c_{12}s_{23} - s_{12}c_{23}s_{13}e^{i\delta_{13}} & c_{23}c_{13} \end{pmatrix} \end{aligned} \quad [13]$$

where $c_{12} = \cos \theta_{12}$, $s_{23} = \sin \theta_{23}$, etc. The requirement that charge–current weak processes are all described by these matrix elements, satisfying the unitarity relation,

$$\sum_\ell U_{i\ell}^{\text{CKM}} U_{\ell k}^{\text{CKM}\dagger} = \delta_{ik} \quad [14]$$

gives a very stringent test for the validity of the model.

CP Violation

CP (product of charge conjugation and parity transformation) invariance is an approximate symmetry of Nature. Although it is known to be broken by very tiny amounts only, the exact extent and the nature of *CP* violation can have far-reaching consequences.

CP violation has first been discovered by Cronin and Fitch (BNL, 1964) in the K -meson system; more precise information on the nature of CP violation from the neutral kaon decays has been obtained more recently (2000) in NA48 (CERN) and KTeV (Fermilab) experiments. CP violation has been established in the B -meson systems as well, very recently (2002), by Babar experiments at SLAC and Belle experiments at KEK.

Through the so-called CPT theorem, CP invariance (or violation) is closely related to the T (time-reversal invariance) symmetry. Also, CP noninvariance is one of the conditions needed in the cosmological baryon number generation (baryogenesis).

In the GWS theory, with three families of quark flavors (six quarks), there is just one source of CP violation: the phase δ_{13} appearing in the CKM matrix (eqn [13]). For $\delta \neq 0, \pi$, W -exchange interactions [12] induce CP violation. The earlier and more recent experimental data on $K^0 - \bar{K}^0$ mixing and $K_{L,S}$ decay data appear to be compatible with the CKM mechanism for CP violation, but a quantitative comparison with the SM remains somewhat hindered by the difficulty of estimating certain strong interaction effects. The recent confirmation of CP violation in B systems is made in the context of a global fit with the SM predictions such as the “unitarity triangle” relations, for example,

$$1 + \frac{U_{ud} U_{ub}^*}{U_{cd} U_{cb}^*} + \frac{U_{td} U_{tb}^*}{U_{cd} U_{cb}^*} = 0 \quad [15]$$

(eqn [14]), and by combining data from kaon decays, charmed meson decays, B meson decay and mixings, etc., and is a part of direct tests of the GWS model, with nonvanishing CP violation CKM

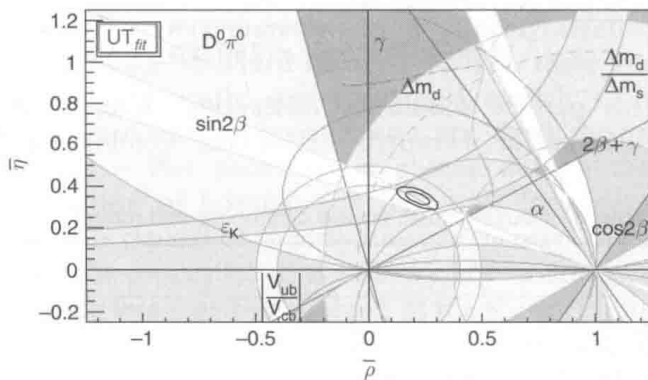


Figure 1 Unitarity triangle test (Eq. (15)). The small ellipses represent 68% and 95% probability zones for the apex corresponding to $U_{ud}U_{ub}^*/U_{cd}U_{cb}^*$. Reproduced from M. Bona *et al.* (2005) The 2004 UTfit collaboration report on the status of the unitarity triangle in the standard model. Journal of High Energy Physics. 0507: 028–059 (hep-ph/0501199), with permission from IoP Publishing Ltd and the UTfit collaboration.

phase (eqn [16] and Figure 1). Recent evidence for nonzero neutrino masses and mixings opens the way to possible CP violation in the leptonic processes as well.

Finally, within the SM including strong interactions, there is one more source of CP violation: the so-called θ (vacuum) parameter of QCD.

B and L Nonconservation

Another set of approximate symmetries in Nature are the baryon and lepton number conservations. In the electroweak theory, these global symmetries are exact to all orders of perturbation theory. Nonperturbative effects (a sort of barrier penetration in gauge field space) however violate both B and L ; the combination $B-L$ is conserved even nonperturbatively though. The nonperturbative electroweak baryon number violation is an extremely tiny effect, the amplitude being proportional to the typical tunneling factor $e^{-2\pi/\alpha}$, but the process is unsuppressed at finite temperatures as might have been experienced by the universe at some early stage after big bang.

B or L nonconservation can also arise naturally at high energy scales, if the electroweak theory is embedded as the low-energy approximation in a grand unified model. The experimental lower limit of proton lifetime, $\tau_p \geq 10^{32}$ years, from Kamio-kande experiments, however severely restricts acceptable models of this type (the simplest $SU(5)$ model is already ruled out).

On the other hand, cosmological baryogenesis requires sufficient amount of baryon number violation, at least in some stage of cosmological expansion. Detailed analyses suggest that the standard electroweak transition might not in itself explain the baryon number $n_p/n_\gamma \sim 10^{-10}$ observed in the present universe. Recent observations of neutrino oscillations suggest the right-handed Majorana-type neutrino masses to be present, which violate the lepton number L . In such a case it might be possible that the correct amount of baryon number excess would be generated, through the leptogenesis.

Global Fit

Various relations exist at the tree level among the masses, scattering cross sections, decay rates, various asymmetries, etc., which can be read off or calculated from the formulas given earlier. These quantities receive corrections at higher orders, and the experimental checks of these modified relations provide precision tests of the model on the one hand, and possibly a hint for new physics, if there is any discrepancy with the prediction. Very often the amplitudes of interest

receive important contributions due to strong interactions, which are difficult to estimate.

The basic parameters of the model, apart from the Higgs mass, and fermion masses and mixing parameters, can be taken to be (1) the fine structure constant, $\alpha = 1/137.035\,999\,11(46)$; (2) the Fermi constant $G_F = 1.166\,37 \times 10^{-5} \text{ GeV}^{-2}$ (which can be determined from the muon lifetime), and the Z-boson mass, $M_Z = 91.1876 \pm 0.0021 \text{ GeV}$ (observed directly at LEP). M_W and $\sin^2 \theta_W$ are then calculable numbers, in terms of these quantities, and depending on m_t (measured independently by CDF and DØ experiments at Fermilab) and on the unknown M_H .

Such precision tests of the GWS model are being made, combining the analyses of various decay rates and asymmetries in B-meson systems at B factories and in colliders, production and decays of Z and W bosons, elastic νe or $\bar{\nu} e$ scatterings, elastic νp or $\bar{\nu} p$ scatterings, deep inelastic lepton nucleon (or deuteron) scatterings, the muon anomalous magnetic moment, atomic parity violation experiments, etc.

An overall fit to the data gives an excellent agreement, with the input parameters

$$M_H = 113^{+56}_{-40} \text{ GeV}, \quad m_t = 176.9 \pm 4.0 \text{ GeV}, \\ \alpha_s(M_Z) = 0.1213 \pm 0.0018$$

For instance (in GeV),

$$M_W = 80.390 \pm 0.018 \text{ vs. } 80.412 \pm 0.042 \\ (\text{exp. value (LEP)}) \\ \Gamma_Z = 2.4972 \pm 0.0012 \text{ vs. } 2.4952 \pm 0.0023 \\ (\text{exp. value})$$

For $\sin^2 \theta_W$ (defined in the so-called \overline{MS} scheme) all data give consistently the value

$$\sin^2 \theta_W = 0.231\,20 \pm 0.000\,15$$

(a slightly larger value is reported by an νN experiment at Fermilab).

The unitarity-triangle tests of the SM and determination of CKM matrix have already been mentioned. The results of global fit can be summarized in Figure 1, and by the angles

$$\begin{aligned} s_{12} &= 0.2243 \pm 0.0016 \\ s_{23} &= 0.0413 \pm 0.0015 \\ s_{13} &= 0.037 \pm 0.0005 \\ \delta_{13} &= 60^\circ \pm 14^\circ \end{aligned} \quad [16]$$

For the muon anomalous gyromagnetic ratio $(g - 2)$, the experimental data

$$a_\mu^{\text{exp}} = \frac{g_\mu - 2}{2} = (1.116\,5920(37) \pm 0.78) \times 10^{-9}$$

is to be compared with the theoretical prediction

$$a_\mu^{\text{th}} = (1.1165918(83) \pm 0.49) \times 10^{-9}$$

which is slightly smaller (1.9σ), where the largest theoretical uncertainty comes from the two-loop hadronic contribution $a_\mu^{\text{had}} \simeq (69.63 \pm 0.72) \times 10^{-9}$ (the QED corrections to $O(\alpha^5)$ are included).

For further details of the analyses and the present status of experimental tests of the electroweak theory, see the reviews by J Erler and P Langacker, and by F J Gilman *et al.*, cited in “Further reading” (most of numbers cited here come from these two reviews).

Need for Extension of the Model

In spite of such an impressive experimental confirmation, there are reasons to believe that the electroweak theory, in its standard minimal form, is not a complete story. As already mentioned, neutrino oscillations, predicted earlier by Pontecorvo, have recently been experimentally confirmed, giving uncontroversial evidence for nonvanishing neutrino masses and their mixing. This is a clear signal that the theory must be extended. If the mass is instead taken in the form of eqn [11] but with three neutrinos families, the diagonalization in general yields a mixing for the light neutrinos, as for the quarks. Some of the experimental data on the neutrinos are summarized in Table 7.

In addition, the Higgs sector of the theory (the part of the interactions responsible for spontaneous breaking $SU_L(2) \times U(1) \rightarrow U_{EM}(1)$) is still largely untested. The theory predicts a physical scalar particle, the Higgs particle, of unknown mass. The present-day expectation for its mass, which combines the experimental lower limit and an indirect upper limit following from the analysis of various radiative corrections, is

$$114 \text{ (GeV)} < m_H < 250 \text{ (GeV)}$$

This particle should be observable either in the Tevatron at Fermilab or in the coming LHC

Table 7 Neutrino mass square differences and mixing

ν_e		ν_μ		ν_τ
$\Delta_{12} m^2$	=	(6 – 9)	×	10^{-5} eV^2
$\Delta_{23} m^2$	=	(1 – 3)	×	10^{-3} eV^2

Solar neutrinos and reactor (SNO, SuperKamiokande, KamLAND) experiments give the first results. Atmospheric neutrino data and the long baseline experiment (SuperKamiokande, K2K) provide the second. The mixing angle relevant to the solar and reactor neutrino oscillation is large, $\tan^2 \theta_{12} \sim 0.40^{+0.10}_{-0.07}$, while the one related to the atmospheric neutrino data is maximal, $\sin^2 2\theta_{23} \sim 1$. Cosmological considerations give $\sum m_{\nu_i} < O(1 \text{ eV})$.

experiments at CERN; negative results would force upon us a substantial modification of the electroweak theory.

Last, but not least, there are a few theoretical motivations for an extension of the model to be considered necessary. First, the structure of the GWS theory is not entirely determined by the gauge principle. The form of the Higgs self-interactions, as well as their number and the Yukawa couplings of the Higgs scalar to the fermions, are unconstrained by any principle, and the particular, minimal form assumed by Weinberg and Salam is yet to be confirmed experimentally.

In addition, the theory is not really a unified gauge theory: $SU_L(2)$ and $U(1)$ gauge couplings are distinct. One possibility is that the $SU(3)_{\text{QCD}} \times SU_L(2) \times U(1)$ theory of the SM is actually a low-energy manifestation of a truly unified gauge theory – grand unified theory (GUT) – defined at some higher mass scale. The simplest version of GUT models based on $SU(5)$ or $SO(10)$ gauge groups has however a difficulty with the proton decay rates, and with the coupling-constant unification itself. Supersymmetric GUTs appear to be more acceptable both from the coupling-constant unification and from the proton lifetime constraints.

A more subtle, but perhaps more severe theoretical problem, is the so-called naturalness problem. At the quantum level, due to the quadratic divergences in the scalar mass, the structure of the theory turns out to be quite peculiar. If the ultraviolet cutoff of the theory is taken to be the Planck mass scale, $\Lambda_{\text{UV}} \sim m_{\text{Pl}} \sim 10^{19} \text{ GeV}$, at which gravity becomes strongly coupled, the theory at Λ_{UV} would have to possess parameters which are fine-tuned with an excessive precision. The problem is known also as a “hierarchy” problem.

A way to avoid having such a difficulty is to introduce supersymmetry. In a supersymmetric version of the standard theory – in fact, there are phenomenologically well-acceptable models such as the minimal supersymmetric standard model (MSSM) – this problem is absent due to the cancellation of bosonic and fermionic loop contributions typical of supersymmetric theories. As a result, the properties of the theory at low energies are much less sensitive to those of the theory at the Planck mass scale. Experiments at LHC (expected to be performed after 2008, CERN) should be able to produce a whole set of new particles associated with supersymmetry, if this is a part of the physical law beyond TeV energies.

At a deeper level, however, the hierarchy problem in a more general sense persists, even in supersymmetric models: why the masses of the order of

$O(100 \text{ GeV})$ should appear at all in a theory with a natural cutoff of the order of the Planck mass? Furthermore, if the masses of the neutrinos turn out to be of the order of $O(10^{-3} - 10^0) \text{ eV}$, we are left with the problem of understanding the large disparities among the quark and lepton masses, spanning the range of more than 13 orders of magnitudes: another “hierarchy” problem.

It is also possible that the spacetime the physical world lives in is actually higher dimensional: the usual four-dimensional Minkowski spacetime times either compactified or uncompactified “extra dimensions.” In theories of this type, some of the difficulties mentioned above might find a natural solution. It is yet to be seen whether a consistent theory of this type can be constructed that correctly account for the properties of the universe we inhabit.

Bibliographic Notes

A short but comprehensive introduction to the Weinberg–Salam theory is found in Taylor (1976); see also Abers and Lee (1973) and 't Hooft and Veltman (1973).

The reprint collection edited by Taylor (2001) contains many of fundamental papers, e.g., on Yang–Mills theories (by CN Yang, RL Mills, R Shaw), on spontaneous symmetry breaking and its application to gauge theories (by Y Nambu, J Schwinger, PW Anderson, PW Higgs, F Englert, R Brout, TWB Kibble) and on renormalization of Yang–Mills theories and application to the electroweak theory (LD Faddeev, VN Popov, G 't Hooft).

For up-to-date review on precision tests of the GWS theory, and details of the analyses, see Erler and Langacker (2004), and references cited therein.

For a recent review on neutrino experiments, see Shirai (2005). For theory on neutrinos, see Fukugita and Yanagida (2003).

For the unitarity triangle test of the GWS model and determination of CKM matrix elements, see results from the CKM fitter Group (Bret *et al.* 2005), the UTfit Collaboration (Bona *et al.* 2005), and a review by Gilman *et al.* (2005), and references cited therein.

See also: Abelian and Nonabelian Gauge Theories using Differential Forms; Current Algebra; Effective Field Theories; Finite Group Symmetry Breaking; Noncommutative Tori, Yang–Mills, and String Theory; Quantum Chromodynamics; Quantum Electrodynamics and Its Precision Tests; Quantum Field Theory: A Brief Introduction; Renormalization: General Theory; Standard Model of Particle Physics; Symmetries and Conservation Laws; Symmetry and Symmetry Breaking in Dynamical Systems; Symmetry Breaking in Field Theory.

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Elliptic Differential Equations: Linear Theory

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Introduction

Motivation: A Model Problem

Many physical problems can be modeled by partial differential equations. Let us consider, for example, the case of an elastic membrane Ω , with fixed boundary Γ , subject to pressure forces f . The vertical membrane displacement is represented by a real-valued function u , which solves the equation

$$-\Delta u(x) = f(x), \quad x = (x_1, x_2) \in \Omega \quad [1]$$

where the Laplace operator Δ is defined, in two dimensions, by

$$\Delta u = \frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2}$$

As the membrane is glued to the curve Γ , u satisfies the condition

$$u(x) = 0, \quad x \in \Gamma \quad [2]$$

The system [1]–[2] is the homogeneous Dirichlet problem for the Laplace operator. It enters the more general framework of (linear) elliptic boundary

value problems, which consist of a (linear) partial differential equation (in the example above, of order two: the highest order in the derivatives) inside an open set Ω of the whole space \mathbb{R}^N , satisfying some “elliptic” property, completed by (linear) conditions on the boundary Γ of Ω , called “boundary conditions.” In the sequel, we only consider the linear case.

Our aim is to answer the following questions: does this problem admit a solution? in which space? is this solution unique? does it depend continuously on the given data f ? In case of positive answers, we say that the problem is “well posed” in the Hadamard sense. But other questions can also be raised, such as the sign of the solution, for example, or its regularity. We give a full survey of linear elliptic problems in a bounded or in an exterior domain with a sufficiently smooth boundary and in the whole space. In the general theory of the elliptic problem, we consider only smooth coefficients. We survey the standard theory, which can be found in the several well-known monographs of the 1960s. The new trends in the investigation of the elliptic problems is to consider more general domains with nonsmooth boundaries and nonsmooth coefficients. On the other hand, the regularity results for elliptic systems have not been improved during last 30 years. New trends also require employment of more general function spaces and more general functional background.

The number of references (see “Further reading” section) is strictly limited here; we list only some of the most important publications. The basic facts can usually be found in more places and sometimes we do not mention the particular reference. Among the

very basic references are Friedman (1969), Gilbarg and Trudinger (1977), Dautray and Lions (1988), Hörmander (1964), Ladyzhenskaya and Ural'tseva (1968), Lions and Magenes (1968), Renardy and Rogers (1992), and Weinberger (1965); of course, there are many others.

The Method

To answer the above questions, we generally use, for such elliptic problems, an approach based on what is called a "variational formulation" (see the section "Variational approach"): the boundary-value problem is first transformed into a variational problem of lower order, which is solved in a Hilbertian frame with help of the Lax–Milgram theorem (based on the representation theorem). All questions are then solved (e.g., existence, uniqueness, continuity in terms of the data, regularity). But this variational formalism does not necessary allow to treat all the situations and it is limited to the Hilbertian case. Other strategies can then be developed, based on *a priori* estimates and duality arguments for the existence problem, or maximum principle for the question of unicity. Without forgetting the particular cases where an explicit Green kernel is computable (e.g., the Laplacian operator in the whole space case).

Moreover, the study of linear elliptic equations is directly linked to the background of function spaces. It is the reason why we first deal with Sobolev spaces – both of the integer and fractional order and we survey their basic properties, imbedding and trace theorems. We pay attention to the Riesz and Bessel potentials and we define weighted Sobolev spaces important in the context of unbounded opens. Second, we present the variational approach and the Lax–Milgram theorem as a key point to solve a large class of boundary-value problems. We give examples: the Dirichlet and Neumann problems for the Poisson equation, the Newton problem for more general second-order operators; we also investigate mixed boundary conditions and present an example of a problem of fourth order. Then, we briefly present the arguments for studying general elliptic problems and concentrate on second-order elliptic problems; we recall the weak and strong maximum principle, formulate the Fredholm alternative and tackle the regularity questions. Moreover, we are interested in the existence and uniqueness of solution of the Laplace equation in the whole space and in exterior opens. Finally, we present some particular examples arising from physical problems, either in fluid mechanics (the Stokes system) or in elasticity.

Sobolev and Other Types of Spaces

Throughout, $\Omega \subset \mathbb{R}^N$ will generally be an open subset of the N -dimensional Euclidean space \mathbb{R}^N .

A domain will be an open and connected subset of \mathbb{R}^N . We shall use standard notations for the spaces $L^p(\Omega)$, $C^\infty(\Omega)$, etc., and their norms. Let us agree that $C^{k,r}(\Omega)$, $k \in \mathbb{N}$, $r \in (0, 1)$, denote the space of functions f in $C^k(\Omega)$, whose derivatives $D^\alpha f$, $\alpha = (\alpha_1, \dots, \alpha_N) \in \mathbb{N}^N$, of order $|\alpha| = \sum_{i=1}^N \alpha_i = k$ are all r -Hölder continuous. In the notations for some of these spaces, by $\bar{\Omega}$ we mean that the functions have the corresponding property on Ω and that they can be continuously extended to $\bar{\Omega}$.

Let us recall several fundamental concepts. The space $\mathcal{D}(\Omega)$ of the test functions in Ω consists of all infinitely differentiable φ with a compact support in Ω . A locally convex topology can be introduced here. The elements of the dual space $\mathcal{D}'(\Omega)$ are called the distributions. If $f \in L^1_{\text{loc}}(\Omega)$ (i.e., $f \in L^1(K)$ for all compact subsets K of Ω), then f is a regular distribution; the duality is represented by $\int_\Omega f(x)\varphi(x)dx$. If $f \in \mathcal{D}'(\Omega)$, we define the distributional or the weak derivative D^α of f as the distribution $\varphi \mapsto (-1)^{|\alpha|} \langle f, D^\alpha \varphi \rangle$. Plainly, if $f \in L^1_{\text{loc}}$ has "classical" partial derivatives in L^1_{loc} , then it coincides with the corresponding weak derivative.

If $\Omega = \mathbb{R}^N$, it is sometimes more suitable to work with the tempered distributions. The role of $\mathcal{D}(\Omega)$ is played by the space $\mathcal{S}(\mathbb{R}^N)$ of C^∞ -functions with finite pseudonorms $\sup |D^\alpha f(x)|(1 + |x|)^k, |\alpha|, k = 0, 1, 2, \dots$. Recall that the Fourier transform \mathcal{F} maps $\mathcal{S}(\mathbb{R}^N)$ into itself and the same is true for the space of the tempered distributions $\mathcal{S}'(\mathbb{R}^N)$.

Sobolev Spaces of Positive Order

The Sobolev space $W^{k,p}(\Omega)$, $1 \leq p \leq \infty$, $k \in \mathbb{N}$, is the space of all $f \in L^p(\Omega)$ whose weak derivatives up to order k are regular distributions belonging to $L^p(\Omega)$; in $W^{k,p}(\Omega)$ we introduce the norm

$$\|f\|_{W^{k,p}(\Omega)} = \left(\sum_{|\alpha| \leq k} \int_\Omega |D^\alpha f(x)|^p dx \right)^{1/p} \quad [3]$$

when $p < \infty$ and $\max_{|\alpha| \leq k} \sup_{x \in \Omega} \text{ess} |D^\alpha f(x)|$ if $p = \infty$. The space $W^{k,p}(\Omega)$ is a Banach space, separable for $p < \infty$ and reflexive for $1 < p < \infty$; it is a Hilbert space for $p = 2$, more simply denoted $H^m(\Omega)$. In the following, we shall consider only the range $p \in (1, \infty)$.

The link with the classical derivatives is given by this well-known fact: a function f belongs to $W^{1,p}(\Omega)$ if and only if it is a.e. equal to a function \tilde{u} , absolutely continuous on almost all line segments in Ω parallel to the coordinate axes, whose (classical) derivatives belong to $L^p(\Omega)$ (the Beppo-Levi theorem).

For $1 < p < \infty$ and noninteger $s > 0$ the Sobolev space $W^{s,p}(\Omega)$ of order s is defined as the space of all f with the finite norm

$$\|f\|_{W^{s,p}(\Omega)} = \left(\|f\|_{W_p^{[s]}(\Omega)}^p + \sum_{|\alpha|=[s]} \int_{\Omega} \int_{\Omega} \frac{|D^{\alpha}f(x) - D^{\alpha}f(y)|^p}{|x-y|^{N+p(s-[s])}} \right)^{1/p}$$

where $[s]$ is the integer part of s (for details, see, e.g., Adams and Fournier (2003) and Ziemer (1989)).

Imbedding Theorems

One of the most useful and important features of the functions in Sobolev spaces is an improvement of their integrability properties and the compactness of various imbeddings. Theorems of this type were first proved by Sobolev and Kondrashev. Let us agree that the symbols \hookrightarrow and $\hookrightarrow\hookrightarrow$ stand for an imbedding and for a compact imbedding, respectively.

Theorem 1 *Let Ω be a Lipschitz open. Then*

- (i) *If $sp < N$, then $W^{s,p}(\Omega) \hookrightarrow L^{p^*}(\Omega)$ with $p^* = Np/(N - ps)$ (the Sobolev exponent). If $|\Omega| < \infty$, then the target space is any $L^r(\Omega)$ with $0 < r \leq p^*$. If Ω is bounded, then $W^{s,p}(\Omega) \hookrightarrow\hookrightarrow L^q(\Omega)$ for all $1 \leq q < p^*$.*
- (ii) *If $sp > N$, then $W^{i+s,p}(\Omega) \hookrightarrow C^i(\Omega)$ for $j=0,1,\dots$. If Ω has the Lipschitz boundary, then $W^{i+s,p}(\Omega) \hookrightarrow C^{i,\mu}(\bar{\Omega})$ for $j=0,1,\dots$ and $\mu = s - N/p$. If $sp > N$, then $W^{i+s,p}(\Omega) \hookrightarrow\hookrightarrow C^i(\Omega)$, $j=0,1,\dots$ and $W^{i+s,p}(\Omega) \hookrightarrow\hookrightarrow W_q^i(\Omega)$ for all $1 \leq q \leq \infty$. If, moreover, Ω has the Lipschitz boundary, then the target space can be replaced by $C^{i,\mu}(\bar{\Omega})$ provided $sp > N > (s-1)p$ and $0 < \mu < s - N/p$.*

Note that if the imbedding $W^{s,p}(\Omega) \hookrightarrow L^q(\Omega)$ is compact for some $q \geq p$, then $|\Omega| < \infty$. Moreover, if $\limsup_{r \rightarrow \infty} |\{x \in \Omega; r \leq |x| < r+1\}| > 0$, then $W^{s,p}(\Omega) \hookrightarrow L^q(\Omega)$ cannot be compact.

Traces and Sobolev Spaces of Negative Order

Let $s > 0$ and let Ω be, for simplicity, a bounded open subset of \mathbb{R}^N with boundary Γ of class $C^{[s],1}$. Then with the help of local coordinates, we can define Sobolev spaces $W^{s,p}(\Gamma)$ (also denoted $H^s(\Gamma)$ for $p=2$) on $\Gamma = \partial\Omega$ (see, e.g., Nečas (1967) and Adams and Fournier (2003) for details). If $f \in C(\bar{\Omega})$, then $f|_{\Gamma}$ has sense. Introducing the space $\mathcal{D}(\bar{\Omega})$ of restrictions in Ω of functions in $\mathcal{D}(\mathbb{R}^N)$, one can show that if $f \in \mathcal{D}(\bar{\Omega})$, we have $\|f|_{\Gamma}\|_{W^{1-1/p,p}(\Gamma)} \leq C\|f\|_{W^{1,p}(\Omega)}$ so that, in view of the density of $\mathcal{D}(\bar{\Omega})$ in $W^{1,p}(\Omega)$, the restriction

of f to Γ can be uniquely extended to the whole $W^{1,p}(\Omega)$. The result is the bounded trace operator $\gamma_0 : W^{1,p}(\Omega) \rightarrow W^{1-1/p,p}(\Gamma)$. Moreover, every $g \in W^{1-1/p,p}(\Gamma)$ can be extended to a (nonunique) function $f \in W^{1,p}(\Omega)$ and this extension operator is bounded with respect to the corresponding norms.

More generally, let us suppose Γ is of class $C^{k-1,1}$ and define the operator Tr_n for any $f \in \mathcal{D}(\bar{\Omega})$ by $\text{Tr}_n f = (\gamma_0 f, \gamma_1 f, \dots, \gamma_{k-1} f)$, where

$$\begin{aligned} \gamma_j f(x) &= \frac{\partial^j f}{\partial n^j}(x) \\ &= \sum_{|\alpha|=j} \frac{j!}{\alpha!} (\partial^{\alpha} f(x) / \partial x^{\alpha}) n^{\alpha}, \quad x \in \Gamma \end{aligned}$$

is the j th-order derivative of f with respect to the outer normal n at $x \in \Gamma$; by density, this operator can be uniquely extended to a continuous linear mapping defined on the space $W^{k,p}(\Omega)$; moreover, $\gamma_0(W^{k,p}(\Omega)) = W^{k-1/p,p}(\Gamma)$.

The kernel of this mapping is the space $\dot{W}^{k,p}(\Omega)$ (denoted by $H_0^k(\Omega)$ for $p=2$), where $\dot{W}^{s,p}(\Omega)$ is defined as the closure of $\mathcal{D}(\Omega)$ in $W^{s,p}(\Omega)$ ($s > 0$). For $1 < p < \infty$, the following holds: $\dot{W}^{s,p}(\mathbb{R}^N) = W^{s,p}(\mathbb{R}^N)$, $\dot{W}^{s,p}(\Omega) = W^{s,p}(\Omega)$ provided $0 < s \leq 1$. If $s < 0$, then the space $W^{s,p}(\Omega)$ is defined as the dual to $\dot{W}^{-s,p'}(\Omega)$, where $p' = p/(p-1)$ (see, e.g., Triebel (1978, 2001)). Observe that, for an arbitrary Ω , a function $f \in W^{1,p}(\Omega)$ has the zero trace if and only if $f(x)/\text{dist}(x, \Gamma)$ belongs to $L^p(\Omega)$.

For $p=2$, we simply denote by $H^{-k}(\Omega)$ the dual space of $H_0^k(\Omega)$. In the case of bounded opens, we recall the following useful Poincaré–Friedrichs inequality (for simplicity, we state it here in the Hilbert frame):

Theorem 2 *Let Ω be bounded (at least in one direction of the space). Then there exists a positive constant $C_P(\Omega)$ such that*

$$\begin{aligned} \|v\|_{L_2(\Omega)} &\leq C_P(\Omega) \|\nabla v\|_{[L_2(\Omega)]^N} \\ \text{for all } v &\in H_0^1(\Omega) \end{aligned} \quad [4]$$

The Whole-Space Case: Riesz and Bessel Potentials

The Riesz potentials \mathcal{I}_{α} naturally occur when one defines the formal powers of the Laplace operator Δ . Namely, if $f \in \mathcal{S}(\mathbb{R}^N)$ and $\alpha > 0$, then

$$\mathcal{F}[(-\Delta)^{\alpha/2} f](\xi) = |\xi|^{\alpha} \mathcal{F}f(\xi).$$

This can be taken formally as a definition of the Riesz potential \mathcal{I}_{α} on $\mathcal{S}'(\mathbb{R}^N)$,

$$\mathcal{I}_{\alpha} f(\cdot) = \mathcal{F}^{-1}[|\xi|^{-\alpha} \mathcal{F}f(\xi)](\cdot)$$

for any $\alpha \in \mathbb{R}$. If $0 < \alpha < N$, then $I_\alpha f(x) = (I_\alpha * f)(x)$, where I_α is the inverse Fourier transform of $|\xi|^{-\alpha}$,

$$I_\alpha(x) = C_\alpha |x|^{\alpha-N}$$

$$C_\alpha = \Gamma((N-\alpha)/2) \left(\pi^{N/2} 2^\alpha \Gamma(\alpha/2) \right)^{-1}$$

where Γ is the Gamma function and I_α is the Riesz kernel. The following formula is also true:

$$I_\alpha(x) = C_\alpha \int_0^\infty t^{(\alpha-N)/2} e^{-\pi|x|^2/t} \frac{dt}{t}$$

Recall that every $f \in \mathcal{S}(\mathbb{R}^N)$ can be represented as the Riesz potential $\mathcal{I}_\alpha g$ of a suitable function $g \in \mathcal{S}(\mathbb{R}^N)$, namely $g = (-\Delta)^{\alpha/2} f$; we get the representation formula

$$\begin{aligned} f(x) &= \mathcal{I}_\alpha g(x) \\ &= C_\alpha \int_{\mathbb{R}^N} \frac{g(y)}{|x-y|^{N-\alpha}} dy \end{aligned}$$

The standard density argument implies then an appropriate statement for functions in $W^{k,p}(\mathbb{R}^N)$ with an integer k and for the Bessel potential spaces $\mathcal{H}^{\alpha,p}(\mathbb{R}^N)$ – see below for their definition. The original Sobolev imbedding theorem comes from the combination of this representation and the basic continuity property of I_α , $\alpha p < N$,

$$I_\alpha: L^p(\mathbb{R}^N) \rightarrow L^q(\mathbb{R}^N), \quad \frac{1}{q} = \frac{1}{p} - \frac{\alpha}{N}$$

To get an isomorphic representation of a Bessel potential space (of a Sobolev space with positive integer smoothness in particular) it is more convenient to consider the Bessel potentials (of order $\alpha \in \mathbb{R}$),

$$\begin{aligned} G_\alpha f(x) &= (G_\alpha * f)(x) \\ &= \mathcal{F}^{-1} \left([1 + |\xi|^2]^{-\alpha/2} \mathcal{F}f(\xi) \right)(x) \end{aligned}$$

(with a slight abuse of the notations); the following formula for the Bessel kernel G_α is well known:

$$G_\alpha(x) = c_\alpha^{-1} \int_0^\infty t^{(\alpha-N)/2} e^{-(\pi|x|^2/t) - (t/4\pi)} \frac{dt}{t}$$

(cf. the analogous formula for I_α), where $c_\alpha = (4\pi)^{\alpha/2} \Gamma(\alpha/2)$. The kernels G_α can alternatively be expressed with help of Bessel or Macdonald functions.

Now we can define the Bessel potential spaces. For $s \in \mathbb{R}$ and $1 < p < \infty$, let $\mathcal{H}^{s,p}(\mathbb{R}^N)$ be the space of all $f \in \mathcal{S}'(\mathbb{R}^N)$ with the finite norm

$$\begin{aligned} \|f\|_{\mathcal{H}^{s,p}(\mathbb{R}^N)} &= \left(\int_{\mathbb{R}^N} \mathcal{F}^{-1} \left((1 + |\xi|^2)^{s/2} \mathcal{F}f(\xi) \right)^p d\xi \right)^{1/p} \end{aligned}$$

In other words, the spaces $\mathcal{H}^{s,p}(\mathbb{R}^N)$ are isomorphic copies of $L^p(\mathbb{R}^N)$.

For $k = 0, 1, 2, \dots$, plainly $\mathcal{H}^{k,2}(\mathbb{R}^N) = W^{k,2}(\mathbb{R}^N)$ by virtue of the Plancherel theorem. But it is true also for integer s and general $1 < p < \infty$ (see, e.g., Triebel (1978)).

Remark 3 Much more comprehensive theory of general Besov and Lizorkin–Triebel spaces in \mathbb{R}^N has been established in the last decades, relying on the Littlewood–Paley theory. Spaces on opens can be defined as restrictions of functions in the corresponding space on the whole \mathbb{R}^N , allowing to derive their properties from those valid for functions on \mathbb{R}^N . The justification for that are extension theorems. In particular, there exists a universal extension operator for the Lipschitz open, working for all the spaces mentioned up to now. We refer to Triebel (1978, 2001).

Unbounded Opens and Weighted Spaces

The study of the elliptic problems in unbounded opens is usually carried out with use of suitable Sobolev weighted space. The Poisson equation

$$-\Delta u = f \quad \text{in } \mathbb{R}^N, \quad N \geq 2 \quad [5]$$

is the typical example; the Poincaré inequality [4] is not true here and it is suitable to introduce Sobolev spaces with weights.

Let $m \in \mathbb{N}$, $1 < p < \infty$, $\alpha \in \mathbb{R}$, $k = m - N/p - \alpha$ if $N/p + \alpha \in \{1, \dots, m\}$ and $k = -1$ elsewhere. For an open $\Omega \subset \mathbb{R}^N$, we define

$$\begin{aligned} W_\alpha^{m,p}(\Omega) &= \left\{ v \in \mathcal{D}'(\Omega), 0 \leq |\lambda| \leq k, \right. \\ &\quad \rho^{\alpha-m-|\lambda|} (\log \rho)^{-1} D^\lambda u \in L^p(\Omega), \\ &\quad k+1 \leq |\lambda| \leq m, \\ &\quad \left. \rho^{\alpha-m+|\lambda|} D^\lambda u \in L^p(\Omega) \right\} \end{aligned}$$

where $\rho(x) = (1 + |x|^2)^{1/2}$. Note that $W_\alpha^{m,p}$ is a reflexive Banach space for the norm $\|\cdot\|_{W_\alpha^{m,p}}$ defined by

$$\begin{aligned} \|u\|_{W_\alpha^{m,p}}^p &= \sum_{0 \leq |\lambda| \leq k} \|\rho^{\alpha-m+|\lambda|} (\log \rho)^{-1} D^\lambda u\|_{L^p(\Omega)}^p \\ &\quad + \sum_{k+1 \leq |\lambda| \leq m} \|\rho^{\alpha-m+|\lambda|} D^\lambda u\|_{L^p(\Omega)}^p \end{aligned}$$

We also introduce the following seminorm:

$$|u|_{W_\alpha^{m,p}} = \left(\sum_{|\lambda|=m} \|\rho^\alpha D^\lambda u\|_{L^p(\Omega)}^p \right)^{1/p}$$

Let

$$\dot{W}_\alpha^{m,p}(\Omega) = \{v \in W_\alpha^{m,p}; \gamma_0(v) = \dots = \gamma_{m-1}(v) = 0\}$$

If Ω is a Lipschitz domain, then $\dot{W}_\alpha^{m,p}(\Omega)$ is the closure of $\mathcal{D}(\Omega)$ in $W_\alpha^{m,p}(\Omega)$, while $\mathcal{D}(\bar{\Omega})$ is dense in $W_\alpha^{m,p}(\Omega)$. We denote by $\dot{W}_\alpha^{-m,p'}(\Omega)$ the dual of $\dot{W}_\alpha^{m,p}(\Omega)$ ($p' = p/(p-1)$). We note that these spaces also contain polynomials,

$$P_j \subset W_\alpha^{m,p}(\Omega) \\ \Leftrightarrow \begin{cases} j = \left[m - \frac{N}{p} - \alpha \right] & \text{if } \frac{N}{p} + \alpha \notin \mathbb{Z} \\ j = m - \frac{N}{p} - \alpha & \text{elsewhere} \end{cases}$$

where $[s]$ is the integer part of s and $P_{[s]} = \{0\}$ if $[s] < 0$. The fundamental property of functions belonging to these spaces is that they satisfy the Poincaré weighted inequality. An open Ω is an exterior domain if it is the complement of a closure of a bounded domain in \mathbb{R}^N .

Theorem 4 Suppose that Ω is an exterior domain or $\Omega = \mathbb{R}_+^N$ or $\Omega = \mathbb{R}^N$. Then

- (i) the seminorm $|\cdot|_{W_\alpha^{m,p}(\Omega)}$ is a norm on $W_\alpha^{m,p}(\Omega)/P_j$, equivalent to the quotient norm with $j' = \min(m-1, j)$;
- (ii) the seminorm $|\cdot|_{W_\alpha^{m,p}(\Omega)}$ is equivalent to the full norm on $\dot{W}_\alpha^{m,p}(\Omega)$.

Variational Approach

Let us first describe the method on the model problem [1]–[2], supposing $f \in L^2(\Omega)$ and Ω bounded. We first suppose that this problem admits a sufficiently smooth function u . Let v be any arbitrary (smooth) function; we multiply eqn [1] by $v(x)$ and integrate with respect to x over Ω ; this gives

$$\int_{\Omega} -(\Delta uv)(x) dx = \int_{\Omega} (fv)(x) dx$$

Using the following Green's formula ($d\sigma(x)$ denotes the measure on $\Gamma = \partial\Omega$ and $\partial u(x)/\partial n = \nabla u(x) \cdot n(x)$, where $n(x)$ is the unit normal at point x of Γ oriented towards the exterior of Ω):

$$\int_{\Omega} (\Delta uv)(x) dx = - \int_{\Omega} (\nabla u \cdot \nabla v)(x) dx + \int_{\Gamma} \left(\frac{\partial u}{\partial n} v \right) (\sigma) d\sigma \quad [6]$$

we get, since $v|_{\Gamma} = 0$: $\mathcal{A}(u, v) = L(v)$, where we have set

$$\begin{aligned} \mathcal{A}(u, v) &= \int_{\Omega} \nabla u(x) \cdot \nabla v(x) dx \\ L(v) &= \int_{\Omega} f(x) v(x) dx \end{aligned} \quad [7]$$

The idea is to study in fact this new problem (showing first its equivalence with the boundary-value problem), noting that it makes sense for far less regular functions u, v (and also f), in fact $u, v \in H_0^1(\Omega)$ (and $f \in H^{-1}(\Omega)$).

The Lax–Milgram Theorem

The general form of a variational problem is

$$\begin{aligned} &\text{to find } u \in V \text{ such that} \\ &\mathcal{A}(u, v) = L(v) \text{ for all } v \in V \end{aligned} \quad [8]$$

where V is a Hilbert space, \mathcal{A} a bilinear continuous form defined on $V \times V$ and L a linear continuous form defined on V . We say, moreover, that \mathcal{A} is V -elliptic if there exists a positive constant α such that

$$\mathcal{A}(u, u) \geq \alpha \|u\|_V^2 \quad \text{for all } u \in V \quad [9]$$

The following theorem is due to Lax and Milgram.

Theorem 5 Let V be a Hilbert space. We suppose that \mathcal{A} is a bilinear continuous form on $V \times V$ which is V -elliptic and that L is a linear continuous form on V . Then the variational problem [8] has a unique solution u on V . Moreover, if \mathcal{A} is symmetric, u is characterized as the minimum value on V of the quadratic functional E defined by

$$\text{for all } v \in V, \quad E(v) = \frac{1}{2} \mathcal{A}(v, v) - L(v) \quad [10]$$

Remark 6

(i) We have the following “energy estimate”: $\|u\|_V \leq \frac{1}{\alpha} \|L\|_{V'}$ where V' is the dual space to V . In the particular case of our model problem, this inequality shows the continuity of the solution $u \in H_0^1(\Omega)$ with respect to the data $f \in L^2(\Omega)$ (that can be weakened by choosing $f \in H^{-1}(\Omega)$).

(ii) Theorem 5 can be extended to sesquilinear continuous forms \mathcal{A} defined on $V \times V$; such a form is called V -elliptic if there exists a positive constant α such that

$$\operatorname{Re} \mathcal{A}(u, u) \geq \alpha \|u\|_V^2 \quad \text{for all } u \in V \quad [11]$$

(iii) Denoting by A the linear operator defined on the space V by $\mathcal{A}(u, v) = \langle Au, v \rangle_{V', V}$, for all $v \in V$, the Lax–Milgram theorem shows that A is an isomorphism from V onto its dual space V' , and the problem [8] is equivalent to solving the equation $Au = L$.

(iv) Let us make some remarks concerning the numerical aspects. First, this variational formulation is the starting point of the well-known finite element method: the idea is to compute a solution of an approximate variational problem stated on a finite subspace of V (leading to the resolution of a linear

system), with a precise control of the error with the exact solution u . Second, the equivalence with a minimization problem allows the use of other numerical algorithms.

Let us now present some classical examples of second-order elliptic problems than can be solved with help of the variational theory.

The Dirichlet Problem for the Poisson Equation

We consider the problem on a bounded Lipschitz open $\Omega \subset \mathbb{R}^N$,

$$\begin{aligned} -\Delta u &= f \\ u &= u_0 \quad \text{on } \Gamma = \partial\Omega \end{aligned} \quad [12]$$

with $u_0 \in H^{1/2}(\Gamma)$, so that there exists $U_0 \in H^1(\Omega)$ satisfying $\gamma_0(U_0) = u_0$. The variational formulation of problem [12] is

$$\begin{aligned} &\text{to find } u \in U_0 + H_0^1(\Omega) \text{ such that} \\ &\text{for all } v \in H_0^1(\Omega), \mathcal{A}(u, v) = L(v) \end{aligned} \quad [13]$$

with \mathcal{A} given by [7] and a more general L with $f \in H^{-1}(\Omega)$, defined by

$$L(v) = \langle f, v \rangle_{H^{-1}(\Omega), H_0^1(\Omega)} \quad [14]$$

The existence and uniqueness of a solution of [13] follows from Theorem 5 (and Poincaré inequality [4]). Conversely, thanks to the density of $\mathcal{D}(\Omega)$ in $H_0^1(\Omega)$, we can show that u satisfies [12]. More precisely, we get:

Theorem 7 *Let us suppose $f \in H^{-1}(\Omega)$ and $u_0 \in H^{1/2}(\Gamma)$; let $U_0 \in H^1(\Omega)$ satisfy $\gamma_0(U_0) = u_0$. Then the boundary-value problem [12] has a unique solution u such that $u - U_0 \in H_0^1(\Omega)$. This is also the unique solution of the variational problem [13]. Moreover, there exists a positive constant $C = C(\Omega)$ such that*

$$\|u\|_{H^1(\Omega)} \leq C(\|f\|_{H^{-1}(\Omega)} + \|u_0\|_{H^{1/2}(\Gamma)}) \quad [15]$$

which shows that u depends continuously on the data f and u_0 .

Moreover, using techniques of Nirenberg's differential quotients, we have the following regularity result (see, e.g., Grisvard (1980)):

Theorem 8 *Let us suppose that Ω is a bounded open subset of \mathbb{R}^N with a boundary of class $C^{1,1}$ and let $f \in L^2(\Omega)$, $u_0 \in H^{3/2}(\Gamma)$. Then $u \in H^2(\Omega)$ and each equation in [12] is satisfied almost everywhere (on Ω for the first one and on Γ for the boundary condition). Moreover, there exists a positive constant $C = C(\Omega)$ such that*

$$\|u\|_{H^2(\Omega)} \leq C(\|f\|_{L^2(\Omega)} + \|g\|_{H^{3/2}(\Gamma)}) \quad [16]$$

By induction, if the data are more regular, that is, $f \in H^k(\Omega)$ and $u_0 \in H^{k+3/2}(\Gamma)$ (with $k \in \mathbb{N}$), and if Γ is of class $C^{k+1,1}$, we get $u \in H^{k+2}(\Omega)$.

Remark 9 Let us point out the importance of the open geometry. For example, if Ω is a bounded plane polygon, one can find $u \in H_0^1(\Omega)$ with $\Delta u \in C^\infty(\bar{\Omega})$, such that $u \notin H^{1+\pi/w}(\Omega)$, where w is the biggest value of the interior angles of the polygon. In particular, if the polygon is not convex, the solution of the Dirichlet problem [12] cannot be in $H^2(\Omega)$.

The Neumann Problem for the Poisson Equation

We consider the problem (n is the unit outer normal on Γ)

$$\begin{aligned} -\Delta u &= f \quad \text{in } \Omega \\ \frac{\partial u}{\partial n} &= h \quad \text{on } \Gamma \end{aligned} \quad [17]$$

Setting $E(\Delta) = \{v \in H^1(\Omega); \Delta v \in L^2(\Omega)\}$, the space $\mathcal{D}(\bar{\Omega})$ is a dense subspace, and we have the following Green formula for all $u \in E(\Delta)$ and $v \in H^1(\Omega)$:

$$\begin{aligned} &\int_{\Omega} \Delta u(x) v(x) dx \\ &= - \int_{\Omega} \nabla u(x) \cdot \nabla v(x) dx + \left\langle \frac{\partial u}{\partial n}, \gamma_0 v \right\rangle_{H^{-1/2}(\Gamma), H^{1/2}(\Gamma)} \end{aligned}$$

If $u \in H^1(\Omega)$ satisfies [17] with $f \in L^2(\Omega)$ and $h \in H^{-1/2}(\Gamma)$, then for any function $v \in H^1(\Omega)$, we have, by virtue of the above Green formula,

$$\begin{aligned} \mathcal{A}(u, v) &= \tilde{L}(v) \\ \tilde{L}v &= \int_{\Omega} f(x) v(x) dx + \langle h, \gamma_0 v \rangle_{H^{-1/2}(\Gamma), H^{1/2}(\Gamma)} \end{aligned}$$

But, here the form \mathcal{A} is not $H^1(\Omega)$ -elliptic; in fact, one can check that, if problem [17] has a solution, then we have necessarily (take $v = 1$ above)

$$\int_{\Omega} f(x) dx + \langle h, 1 \rangle_{H^{-1/2}(\Gamma), H^{1/2}(\Gamma)} = 0 \quad [18]$$

Moreover, we note that if u is a solution, then $u + C$, where C is an arbitrary constant, is also a solution. So the variational problem is not well posed on $H^1(\Omega)$. It can, however, be solved in the quotient space $H^1(\Omega)/\mathbb{R}$, which is a Hilbert space for the quotient norm

$$\|v\|_{H^1(\Omega)/\mathbb{R}} = \inf_{k \in \mathbb{R}} \|v + k\|_{H^1(\Omega)} \quad [19]$$

but also for the seminorm $v \mapsto |v|_{H^1(\Omega)} = \sqrt{\mathcal{A}(v, v)}$, which is an equivalent norm on this quotient space (see Nečas (1967)).

Then, supposing that the data f and h satisfy the “compatibility condition” [18], we can apply the Lax–Milgram theorem to the variational problem

$$\begin{aligned} &\text{to find } \dot{u} \in V \text{ such that} \\ &\mathcal{A}(\dot{u}, \dot{v}) = \tilde{L}(\dot{v}) \text{ for all } \dot{v} \in V \end{aligned} \quad [20]$$

with $V = H^1(\Omega)/\mathbb{R}$. We get the following result (see, e.g., Nečas (1967)):

Theorem 10 *Let us suppose that Ω is connected and that the data $f \in L^2(\Omega)$ and $h \in H^{-1/2}(\Gamma)$ satisfy [18]. Then the variational problem [20] has a unique solution \dot{u} in the space $H^1(\Omega)/\mathbb{R}$ and this solution is continuous with respect to the data, that is, there exists a positive constant $C = C(\Omega)$ such that*

$$\begin{aligned} \|u\|_{H^1(\Omega)} &\leq C(\|f\|_{L^2(\Omega)} + \|h\|_{H^{-1/2}(\Gamma)}) \\ &\text{for all } u \in \dot{u} \end{aligned}$$

Moreover, if Γ is of class $C^{1,1}$ and if the data satisfy $f \in L^2(\Omega)$, $g \in H^{1/2}(\Gamma)$, then every $u \in \dot{u}$ is such that $u \in H^2(\Omega)$ and it satisfies each equation in [17] almost everywhere.

Problem with Mixed Boundary Conditions

Here we consider more general boundary conditions: the Dirichlet conditions on a closed subset Γ_1 of $\Gamma = \partial\Omega$, and the Neumann, or more generally the “Robin”, conditions on the other part $\Gamma_2 = \Gamma - \Gamma_1$. We seek u such that ($f \in L^2(\Omega)$, $h \in L^2(\Gamma_2)$, $a \in L^\infty(\Gamma_2)$)

$$\begin{aligned} -\Delta u &= f \quad \text{in } \Omega \\ u &= 0 \quad \text{on } \Gamma_1 \\ au + \frac{\partial u}{\partial n} &= h \quad \text{on } \Gamma_2 \end{aligned} \quad [21]$$

Let $V = \{v \in H^1(\Omega); \gamma_0 v = 0 \text{ on } \Gamma_1\}$. Then [8] is the variational formulation of this problem with

1. $\mathcal{A}(u, v) = \int_{\Omega} \nabla u(x) \cdot \nabla v(x) dx + \int_{\Gamma_2} (a\gamma_0 u \gamma_0 v)(\sigma) d\sigma$;
2. $L(v) = \int_{\Omega} f(x)v(x) dx + \int_{\Gamma_2} (h\gamma_0 v)(\sigma) d\sigma$.

Supposing, for example, $a \geq 0$, we get a unique solution $u \in V$ for this variational problem by virtue of the Lax–Milgram theorem. Moreover, if $u \in H^2(\Omega)$, then u is the unique solution in $H^2(\Omega) \cap V$ of the problem [21].

The Newton Problem for More General Operators

Let Ω be a bounded open subset of \mathbb{R}^n . We now consider more general second-order operators of the form $v \mapsto -\nabla \cdot (M \nabla v) + b \cdot \nabla v + cv$, where $b \in$

$[W^{1,\infty}(\Omega)]^N$, $c \in L^\infty(\Omega)$, M is an $N \times N$ square matrix with entries M_{ij} , and $\nabla \cdot (M \nabla v)$ stands for

$$\sum_{i,j=1}^N \frac{\partial}{\partial x_i} \left[M_{ij} \frac{\partial u}{\partial x_j} \right]$$

We also assume that there is a positive constant α_M such that

$$\begin{aligned} \sum_{i,j=1}^N M_{ij}(x) \xi_i \xi_j &\geq \alpha_M \sum_{i=1}^N \xi_i^2 \\ &\text{for a.e. } x \in \Omega \text{ and } \xi = (\xi_1, \dots, \xi_N) \in \mathbb{R}^N \end{aligned}$$

For given data $f \in L^2(\Omega)$, $h \in L^2(\Gamma)$, we look for a solution u of the problem

$$\begin{aligned} -\nabla \cdot (M \nabla u) + b \cdot \nabla u + cu &= f \quad \text{in } \Omega \\ au + n \cdot (M \nabla u) &= h \quad \text{on } \Gamma \end{aligned} \quad [22]$$

We assume that $a \in L^\infty(\Gamma)$. The variational formulation of this problem is still [8], with $V = H^1(\Omega)$ and

$$\begin{aligned} \mathcal{A}(u, v) &= \int_{\Omega} M \nabla u \cdot \nabla v dx \\ &+ \int_{\Omega} [b \cdot \nabla u + cu] v dx + \int_{\Gamma} a \gamma_0 u \gamma_0 v d\sigma \end{aligned} \quad [23]$$

$$L(v) = \int_{\Omega} f(x)v(x) dx + \int_{\Gamma} (h\gamma_0 v)(\sigma) d\sigma \quad [24]$$

If the conditions

$$\begin{aligned} c - \frac{1}{2} \nabla \cdot b &\geq C_0 \geq 0 \quad \text{a.e. on } \Omega \\ a + \frac{1}{2} b \cdot \nu &\geq C_1 \geq 0 \quad \text{a.e. on } \Gamma \end{aligned}$$

are fulfilled, with $(C_0, C_1) \neq (0, 0)$, then the bilinear form \mathcal{A} is V -elliptic and the Lax–Milgram theorem applies.

A Biharmonic Problem

We consider the Dirichlet problem for the operator of fourth order: ($c \in L^\infty(\Omega)$):

$$\Delta^2 u + cu = f \quad \text{in } \Omega \quad [25]$$

$$u = u_0 \text{ on } \Gamma, \quad \frac{\partial u}{\partial n} = h \text{ on } \Gamma \quad [26]$$

Theorem 11 *Let us suppose that Ω has a boundary of class $C^{1,1}$ and that the data satisfy $f \in H^{-2}(\Omega)$, $u_0 \in H^{3/2}(\Gamma)$, $h \in H^{1/2}(\Gamma)$. Let $U_0 \in H^2(\Omega)$ be such that $\gamma_0(U_0) = u_0$, $\gamma_1(U_0) = h$. Then, if $c \geq 0$ a.e. in Ω , the boundary value problem [25]–[26] has a unique*

solution u such that $u - U_0 \in H_0^2(\Omega)$, and u is also the unique solution of the variational problem

$$\begin{aligned} &\text{to find } u \in U_0 + H_0^2(\Omega) \text{ such that} \\ &A(u, v) = l(v) \text{ for all } v \in H_0^2(\Omega) \end{aligned} \quad [27]$$

where $l(v) = \langle f, v \rangle_{H^{-2}(\Omega), H_0^2(\Omega)}$ and

$$A(u, v) = \int_{\Omega} \Delta u(x) \Delta v(x) dx + \int_{\Omega} (cu v)(x) dx \quad [28]$$

Moreover, there exists a positive constant $C = C(\Omega)$ such that

$$\begin{aligned} \|u\|_{H^2(\Omega)} &\leq C [\|f\|_{H^{-2}(\Omega)} + \|u_0\|_{H^{3/2}(\Gamma)} \\ &\quad + \|b\|_{H^{1/2}(\Gamma)}] \end{aligned} \quad [29]$$

which shows that u depends continuously upon the data f , u_0 , and b .

Remark 12 The Hilbert space choice V is of crucial importance for the V -ellipticity. In fact, let us consider for example the problem [25], with

$$\Delta u = 0 \text{ on } \Gamma, \quad \frac{\partial \Delta u}{\partial n} = 0 \text{ on } \Gamma \quad [30]$$

In fact, the associated bilinear form is not V -elliptic for $V = H^2(\Omega)$ but it is V -elliptic for $V = \{v \in L^2(\Omega); \Delta v \in L^2(\Omega)\}$.

General Elliptic Problems

Here Ω will be a bounded and sufficiently regular open subset of \mathbb{R}^N . Let us consider a general linear differential operator of the form

$$A(x, D)u = \sum_{|\mu| \leq l} a_{\mu}(x) D^{\mu} u, \quad a_{\mu}(x) \in \mathbb{C} \quad [31]$$

Setting $A_0(x, \xi) = \sum_{|\mu|=l} a_{\mu}(x) \xi^{\mu}$, we say that the operator A is elliptic at a point x if $A_0(x, \xi) \neq 0$ for all $\xi \in \mathbb{R}^N - \{0\}$. One can show that, if $N \geq 3$, l is even, that is, $l = 2m$; the same result holds for $N = 2$ if the coefficients a_{μ} are real. Moreover, for $N \geq 3$, every elliptic operator is properly elliptic, in the following sense: for any independent vectors ξ, ξ' in \mathbb{R}^N , the polynomial $\tau \mapsto A_0(\cdot, \xi + \tau \xi')$ has m roots with positive imaginary part.

The aim here is to study boundary-value problems of the following type:

$$Au = f \quad \text{in } \Omega \quad [32]$$

$$B_j u = g_j \quad \text{on } \Gamma, \quad j = 0, \dots, m-1, \quad [33]$$

where A is properly elliptic on $\bar{\Omega}$, with sufficiently regular coefficients, and the operators B_j are boundary operators, of order $m_j \leq 2m - 1$, that must

satisfy some compatibility conditions with respect to the operator A (see Renardy and Rogers (1992) for details; these conditions were introduced by Agmon, Douglis, and Nirenberg). For example, $A = (-1)^m \Delta^m$ and $B_j = \partial^j / \partial n^j$ is a convenient choice.

In order to show that problem [32]–[33] has a solution $u \in H^{2m+r}(\Omega)$ ($r \in \mathbb{N}$), the idea is to show that the operator \mathcal{P} defined by $u \mapsto \mathcal{P}(u) = (Au, B_0 u, \dots, B_{m-1} u)$ is an index operator from $H^{2m+r}(\Omega)$ into $G = H^r(\Omega) \times \prod_{j=0}^{m-1} H^{2m+r-m_j-1/2}(\Gamma)$ and to express the compatibility conditions through the adjoint problem.

We recall that a linear continuous operator \mathcal{P} is an index operator if

- (1) $\dim \text{Ker } \mathcal{P} < \infty$, and $\text{Im } \mathcal{P}$ closed;
- (2) $\text{codim Im } \mathcal{P} < \infty$.

Then the index $\chi(\mathcal{P})$ is given by $\chi(\mathcal{P}) = \dim \text{Ker } \mathcal{P} - \text{codim Im } \mathcal{P}$. We recall the following Peetre's theorem:

Theorem 13 Let E, F , and G be three reflexive Banach spaces such that $E \hookrightarrow F$, and \mathcal{P} a linear continuous operator from E to G . Then condition (1) is equivalent to: "there exists $C \geq 0$, such that for all $u \in E$, we have $\|u\|_E \leq C(\|\mathcal{P}u\|_G + \|u\|_F)$."

Applying this theorem to our problem [32]–[33], condition (1) results from *a priori* estimates of the following type:

$$\|u\|_{H^{2m+r}(\Omega)} \leq C (\|\mathcal{P}u\|_G + \|u\|_{H^{2m+r-1}(\Omega)})$$

and condition (2) by similar *a priori* estimates for the dual problem.

Second-Order Elliptic Problems

We consider a second-order differential operator of the "divergence form"

$$Au = - \sum_{i,j=1}^N (a^{ij}(x) u_{x_i})_{x_j} + \sum_{i=1}^N b^i(x) u_{x_i} + c(x) u \quad [34]$$

with given coefficient functions a^{ij}, b^i, c ($i, j = 1, \dots, N$), and where we have used the notation $u_{x_i} = \frac{\partial u}{\partial x_i}$. Such operators are said uniformly strongly elliptic in Ω if there exists $\alpha > 0$ such that

$$\sum_{|i|=|j|=1} a^{ij}(x) \xi^i \xi^j \geq \alpha |\xi|^2 \quad \text{for all } x \in \Omega, \xi \in \mathbb{R}^N$$

Remark 14 There exist elliptic problems for which the associated variational problem does not necessarily satisfy the ellipticity condition. Let us consider

the following example, due to Seeley: let $\Omega = \{(r, \theta) \in (\pi, 2\pi) \times [0, 2\pi]\}$ and

$$A = -\left(e^{i\theta} \frac{\partial}{\partial \theta}\right)^2 - e^{2i\theta} \left(1 + \frac{\partial^2}{\partial r^2}\right)$$

One can check that, for all $\lambda \in \mathbb{C}$, the problem $Au + \lambda u = f$ in Ω and $u = 0$ on Γ admits nonzero solutions u which are given by (with μ such that $\mu^2 = \lambda$) $u = \sin r \cos(\mu e^{-i\theta})$ and $u = \sin r \sin(\mu e^{-i\theta})$ for $\lambda \neq 0$; $u = \sin r$ and $u = \sin \theta e^{-i\theta}$ for $\lambda = 0$.

Most of the results concerning existence, unicity, and regularity for second-order elliptic problems can be established thanks to a maximum principle. There exist different types of maximum principles, which we now present.

Maximum Principle

Theorem 15 (Weak maximum principle). *Let A be a uniformly strongly elliptic operator of the form [34] in a bounded open $\Omega \subset \mathbb{R}^N$, with $a^{ij}, b^i, c \in L^\infty(\Omega)$ and $c \geq 0$. Let $u \in C^2(\Omega) \cap C(\bar{\Omega})$ and*

$$Au \geq 0 \text{ [resp. } Au \leq 0] \text{ in } \Omega$$

Then

$$\inf_{\Omega} u \geq \inf_{\partial\Omega} u^- \text{ [resp. } \sup_{\Omega} u \leq \sup_{\partial\Omega} u^+]$$

where $u^+ = \max(u, 0)$ and $u^- = -\min(u, 0)$. If $c = 0$ in Ω , one can replace u^- [resp. u^+] by u .

Theorem 16 (Strong principle maximum). *Under the assumptions of the above theorem, if u is not a constant function in $C^2(\Omega) \cap C(\bar{\Omega})$ such that $Au \geq 0$ [resp. $Au \leq 0$], then $\inf_{\Omega} u < u(x)$ [resp. $\sup_{\Omega} u > u(x)$], for all $x \in \Omega$.*

Remark 17 These two maximum principles can be adapted to elliptic operators in nondivergence form, that is,

$$Au = - \sum_{i,j=1}^N a^{ij}(x) u_{x_i x_j} + \sum_{i=1}^N b^i(x) u_{x_i} + c(x) u \quad [35]$$

Fredholm Alternative

We now present some existence results which are based on the Fredholm alternative rather than on the variational method.

Let us consider two Hilbert spaces V and H , where V is a dense subspace of H and $V \hookrightarrow H$. Denoting by V' the dual space of V , and identifying H with its dual space, we have the following imbeddings: $V \hookrightarrow H \hookrightarrow V'$. Let \mathcal{A} be a sesquilinear

form on $V \times V$, V -coercive with respect to H , that is, there exist $\lambda_0 \in \mathbb{R}$ and $\alpha > 0$ such that

$$\operatorname{Re}(\mathcal{A}(v, v)) + \lambda_0 \|v\|_H^2 \geq \alpha \|v\|_V^2 \quad \text{for all } v \in V$$

Denoting by A the operator associated with the bilinear form \mathcal{A} (see Remark 6(iii)), the equation $Au = f$ is equivalent to $u - \lambda_0 T u = g$, with $T = (A + \lambda_0 \operatorname{Id})^{-1}$ and $g = T f$. Note that T is an isomorphism from H onto $D(A) = \{u \in H; Au \in H\}$.

The operator $T: H \rightarrow H$ is compact and, thanks to the Fredholm alternative, there are two situations:

1. either $\operatorname{Ker} A = 0$ and A is an isomorphism from $D(A)$ onto H ;
2. or $\operatorname{Ker} A \neq 0$; then $\operatorname{Ker} A$ is of finite dimension, and the problem $Au = f$ with $f \in H$ admits a solution if and only if $f \in \operatorname{Im} A = [\operatorname{Ker}(A^*)]^\perp$.

We now give another example in a non-Hilbertian frame. Let us consider the problem (Grisvard 1980): $Au = f$ in Ω and $Bu = g$ on Γ , where Γ is of class $C^{1,1}$, A , which is defined by [34], is uniformly strongly elliptic with $a^{ij} = a^{ji} \in C^{0,1}(\bar{\Omega})$, $b^i, c \in L^\infty(\Omega)$, and $Bu = \gamma_0(u)$ or $Bu = \gamma_1(u)$. One can show that the operator $u \mapsto (Au, Bu)$ is a Fredholm operator of index zero from $W^{2,p}(\Omega)$ in $L^p(\Omega) \times W^{2-d-1/p,p}(\Gamma)$ (with $d=0$ if $Bu = \gamma_0(u)$ and $d=1$ if $Bu = \gamma_1(u)$).

Regularity

Assume that Ω is a bounded open. Suppose that $u \in H_0^1(\Omega)$ is a weak solution of the equation

$$\begin{aligned} Au &= f & \text{in } \Omega \\ u &= 0 & \text{on } \Gamma \end{aligned} \quad [36]$$

where A has the divergence form [34]. We now address the question whether u is in fact smooth: this is the regularity problem for weak solutions.

Theorem 18 (H^2 -regularity). *Let Ω be open, of class $C^{1,1}$, $a^{ij} \in C^1(\bar{\Omega})$, $b^i, c \in L^\infty(\Omega)$, $f \in L^2(\Omega)$. Suppose, furthermore, that $u \in H^1(\Omega)$ is a weak solution of [36]. Then $u \in H^2(\Omega)$ and we have the estimate*

$$\|u\|_{H^2(\Omega)} \leq C(\|f\|_{L^2(\Omega)} + \|u\|_{L^2(\Omega)})$$

where the constant C depends only on Ω and on the coefficients of A .

Theorem 19 (Higher regularity). *Let m be a non-negative integer, Ω be open, of class $C^{m+1,1}$ and assume that $a^{ij} \in C^{m+1}(\bar{\Omega})$, $b^i, c \in C^{m+1}(\bar{\Omega})$, $f \in H^m(\Omega)$. Suppose, furthermore, that $u \in H^1(\Omega)$ is a weak solution of [36]. Then $u \in H^{m+2}(\Omega)$ and*

$$\|u\|_{H^{m+2}(\Omega)} \leq C(\|f\|_{H^m(\Omega)} + \|u\|_{L^2(\Omega)})$$

where the constant C depends only on Ω and on the coefficients of A . In particular, if $m > N/2$, then $u \in C^2(\bar{\Omega})$. Moreover, if Ω is of C^∞ class and $f \in C^\infty(\bar{\Omega})$, $a^{ij} \in C^\infty(\bar{\Omega})$, $b^i, c \in C^\infty(\bar{\Omega})$, then $u \in C^\infty(\bar{\Omega})$.

Remark 20

- (i) If $u \in H_0^1(\Omega)$ is the unique solution of [36], one can omit the L^2 -norm of u in the right-hand side of the above estimate.
- (ii) Moreover, let us suppose the coefficients a^{ij}, b^i and c are all C^∞ and $f \in C^\infty(\Omega)$; then, if $u \in H^1(\Omega)$ satisfies $Au = f, u \in C^\infty(\Omega)$; this is due to the "hypoellipticity" property satisfied by the operator A .

We have a similar result in the L^p frame (Grisvard 1980):

Theorem 21 ($W^{2,p}$ -regularity). *Let Ω be open, of class $C^{1,1}$, $a^{ij} \in C^1(\bar{\Omega})$, $b^i, c \in L^\infty(\Omega)$. Suppose, furthermore, that $b^i = 0, 1 \leq i \leq N$ and $c \geq 0$ a.e. Then for every $f \in L^p(\Omega)$ there exists a unique solution $u \in W^{2,p}(\Omega)$ of [36].*

Unbounded Open

The Whole Space

Note in passing that we shall work with the weighted Sobolev spaces $W_\alpha^{m,p}(\Omega)$ defined in the subsection "Unbounded opens and weighted spaces."

Theorem 22 *The following claims hold true:*

- (i) Let $f \in W_0^{-1,p}(\mathbb{R}^N)$ satisfy the compatibility condition

$$\langle f, 1 \rangle_{W_0^{-1,p}(\mathbb{R}^N) \times W_0^{1,p'}(\mathbb{R}^N)} = 0 \quad \text{if } p' \geq N$$

Then the problem [5] has a solution $u \in W_0^{1,p}(\mathbb{R}^N)$, which is unique up to an element in $\mathcal{P}_{[1-N/p]}$ and satisfies the estimate

$$\|u\|_{W_0^{1,p}(\mathbb{R}^N)/\mathcal{P}_{[1-N/p]}} \leq C\|f\|_{W_0^{-1,p}(\mathbb{R}^N)}$$

Moreover, if $1 < p < N$, then $u = E * f$.

- (ii) If $f \in L^p(\mathbb{R}^N)$, then the problem [5] has a solution $u \in W_0^{2,p}(\mathbb{R}^N)$, which is unique up to an element in $\mathcal{P}_{[2-N/p]}$ and if $1 < p < N/2$, then $u = E * f$.

The Calderón–Zygmund inequality

$$\left\| \frac{\partial^2 \varphi}{\partial x_i \partial x_j} \right\|_{L^p(\mathbb{R}^N)} \leq C(N, p) \|\Delta \varphi\|_{L^p(\mathbb{R}^N)}$$

$$\varphi \in \mathcal{D}(\mathbb{R}^N)$$

and Theorem 4 are crucial for establishing Theorem 22.

Further, point (i) means that the Riesz potential of second order satisfies

$$I_2: W_0^{-1,p}(\mathbb{R}^N) \perp \mathcal{P}_{[1-N/p]} \rightarrow W_0^{1,p}(\mathbb{R}^N)/\mathcal{P}_{[1-N/p]}$$

(where the initial space is the orthogonal complement of $\mathcal{P}_{[1-N/p]}$ in $W_0^{-1,p}(\mathbb{R}^N)$) and it is an isomorphism.

Note that here

$$W_0^{1,p}(\mathbb{R}^N) = \{v \in L^{p^*}(\mathbb{R}^N); \nabla v \in L^p(\mathbb{R}^N)\}$$

for $1 < p < N$ and $1/p^* = 1/p - 1/N$. And for $1 < r < N/2$, we also have the continuity property

$$I_2: L^r(\mathbb{R}^N) \rightarrow L^q(\mathbb{R}^N), \quad \text{for } \frac{1}{q} = \frac{1}{r} - \frac{2}{N}$$

Remark 23 The problem

$$u - \Delta u = f \quad \text{in } \mathbb{R}^N \quad [37]$$

is of a completely different nature than the problem [5]. The class of function spaces appropriate for the problem [37] are the classical Sobolev spaces. With the help of the Calderón–Zygmund theory, one can prove that if $f \in L^p(\mathbb{R}^N)$, then the unique solution of [37] belongs to $W^{2,p}(\mathbb{R}^N)$ and can be represented as the Bessel potential of second order (see Stein (1970)): $u = G * f$, where G is the appropriate Bessel kernel, that is, G , for which $\hat{G}(\xi) \sim (1 + |\xi|^2)^{-1/2}$. Recall that in particular $G(x) \sim |x|^{-1} e^{-|x|}$ for $N = 3$. In the Hilbert case, $f \in L^2(\mathbb{R}^N)$, we get

$$(1 + |\xi|^2) \hat{u} \in L^2(\mathbb{R}^N)$$

which, by Plancherel's theorem, implies that $u \in H^2(\mathbb{R}^N)$. For $f \in W^{-1,p}(\mathbb{R}^N)$, the problem [37] has a unique solution $u \in W^{1,p}(\mathbb{R}^N)$ satisfying the estimate

$$\|u\|_{W^{1,p}(\mathbb{R}^N)} \leq C(p, n) \|f\|_{W^{-1,p}(\mathbb{R}^N)}$$

Exterior Domain

We consider the problem in an exterior domain with the Dirichlet boundary condition

$$\begin{aligned} -\Delta u &= f \quad \text{in } \Omega \\ u &= g \quad \text{on } \Gamma = \partial\Omega \end{aligned} \quad [38]$$

where $f \in W_0^{-1,p}(\Omega)$ and $g \in W^{1-1/p,p}(\partial\Omega)$. Invoking the results for \mathbb{R}^N and bounded domains, one can prove the existence of a solution $u \in W_0^{1,p}(\Omega)$ which is unique up to an element of the kernel $A_0^p(\Omega) = \{z \in$

$W_0^{1,p}(\Omega; \Delta z=0)$ provided that f satisfies the compatibility condition

$$\langle f, \varphi \rangle = \left\langle g, \frac{\partial \varphi}{\partial n} \right\rangle \quad \text{for all } \varphi \in A_0^{p'}(\Omega)$$

The kernel can be characterized in the following way: it is reduced to $\{0\}$ if $p=2$ or $p < N$ and if not, then

$$A_0^p(\Omega) = \{C(\lambda - 1); C \in \mathbb{R}\} \quad \text{if } p \geq N \geq 3$$

where λ is (unique) solution in $W_0^{1,2}(\Omega) \cap W_0^{1,p}(\Omega)$ of the problem $\Delta \lambda = 0$ in Ω and $\lambda = 1$ on $\partial\Omega$, and

$$A_0^p(\Omega) = \{C(\mu - u_0); C \in \mathbb{R}\} \quad \text{if } p > N = 2$$

where $u_0(x) = (2\pi|\Gamma|)^{-1} \int_{\Gamma} \log|y-x| d\sigma_y$ and μ is the only solution in $W_0^{1,2}(\Omega) \cap W_0^{1,p}(\Omega)$ of the problem $\Delta \mu = 0$ in Ω and $\mu = u_0$ on Γ .

Remark 24 Similar results exist for the Neumann problem in an exterior domain (see Amrouche *et al.* (1997)). The framework of the spaces $W_{\alpha}^{m,p}(\mathbb{R}_+^N)$ for the Dirichlet problem in \mathbb{R}_+^N was also considered in the literature. For a more general theory see Kozlov and Maz'ya (1999).

Elliptic Systems

The Stokes System

The Stokes problem is a classical example in the fluid mechanics. This system models the slow motion with the field of the velocity \mathbf{u} and the pressure π , satisfying

$$\begin{aligned} (S) \quad & -\nu \Delta \mathbf{u} + \nabla \pi = \mathbf{f} \quad \text{in } \Omega \\ & \operatorname{div} \mathbf{u} = h \quad \text{in } \Omega \\ & \mathbf{u} = \mathbf{g} \quad \text{on } \Gamma = \partial\Omega \end{aligned}$$

where $\nu > 0$ denotes the viscosity, \mathbf{f} is an exterior force, \mathbf{g} is the velocity of the fluid on the domain boundary, and h measures the compressibility of the fluids (if $h=0$, it is an incompressible fluid). The functions h and \mathbf{g} must satisfy the compatibility condition

$$\int_{\Omega} h(x) dx = \int_{\Gamma} \mathbf{g} \cdot \mathbf{n} d\sigma \quad [39]$$

Theorem 25 Let Ω be a Lipschitz bounded domain in \mathbb{R}^N , $N \geq 2$. Let $\mathbf{f} \in H^{-1}(\Omega)^N$, $h \in L^2(\Omega)$, and $\mathbf{g} \in H^{1/2}(\Gamma)^N$ satisfy [39]. Then the problem (S) has a unique solution $(\mathbf{u}, \pi) \in H^1(\Omega)^N \times L^2(\Omega)/\mathbb{R}$ satisfying the a priori estimate

$$\begin{aligned} & \|\mathbf{u}\|_{H^1(\Omega)} + \|\pi\|_{L^2(\Omega)/\mathbb{R}} \\ & \leq C(\|\mathbf{f}\|_{H^{-1}(\Omega)} + \|h\|_{L^2(\Omega)} + \|\mathbf{g}\|_{H^{1/2}(\Gamma)}) \end{aligned}$$

In order to prove Theorem 25, one can start with a homogeneous problem. The procedure of finding \mathbf{u} is a simple application of the Lax–Milgram theorem. Application of de Rham's theorem gives the pressure π . We introduce the space

$$\mathcal{V} = \{\mathbf{v} \in \mathcal{D}(\Omega)^N; \operatorname{div} \mathbf{v} = 0\}$$

and define $\mathbf{F} \in H^{-1}(\Omega)^N$ by

$$\langle \mathbf{F}, \mathbf{v} \rangle_{H^{-1} \times \dot{H}^1} = 0 \quad \text{for all } \mathbf{v} \in \mathcal{V}$$

Moreover, there exists $\pi \in L^2(\Omega)$, unique up to an additive constant, and such that $\mathbf{F} = \nabla \pi$. The problem (S), which we transform to the homogeneous case ($h=0, \mathbf{g}=0$), can be formulated on an abstract level. Let X and M be two real Hilbert spaces and consider the following variational problem: Given $L \in X'$ and $X \in M'$, find $(\mathbf{u}, \pi) \in X \times M$ such that

$$\begin{aligned} \mathcal{A}(\mathbf{u}, \mathbf{v}) + B[\mathbf{v}, \pi] &= L(\mathbf{v}), \quad \mathbf{v} \in X \\ B[\mathbf{u}, q] &= X(q), \quad q \in M \end{aligned} \quad [40]$$

where the bilinear forms \mathcal{A}, B and the linear form L are defined by

$$\begin{aligned} \mathcal{A}(\mathbf{u}, \mathbf{v}) &= \int_{\Omega} \nabla \mathbf{u} \cdot \nabla \mathbf{v} \\ B[\mathbf{v}, q] &= - \int_{\Omega} [q \nabla \cdot \mathbf{v}] \\ L(\mathbf{v}) &= \int_{\Omega} \mathbf{f} \cdot \mathbf{v} \end{aligned}$$

Theorem 26 If the bilinear form \mathcal{A} is coercive in the space

$$V = \{\mathbf{v} \in X; B[\mathbf{v}, q] = 0\} \quad \text{for all } q \in M$$

that is, if there exists $\alpha > 0$ such that

$$\mathcal{A}(\mathbf{v}, \mathbf{v}) \geq \alpha \|\mathbf{v}\|_X^2, \quad \mathbf{v} \in V$$

then the problem [40] has a unique solution (\mathbf{u}, π) if and only if the bilinear form B satisfies the “inf–sup” condition:

there exists $\beta > 0$ such that

$$\inf_{q \in M} \sup_{\mathbf{v} \in X} \frac{B(\mathbf{v}, q)}{\|\mathbf{v}\|_X \|q\|_M} \geq \beta$$

As for the Dirichlet problem, the regularity result is the following:

Theorem 27 Let Ω be a bounded domain in \mathbb{R}^N , of the class $C^{m+1,1}$ if $m \in \mathbb{N}$ and $C^{1,1}$ if $m = -1$. Let $\mathbf{f} \in W^{m,p}(\Omega)^N$, $h \in W^{m+1,p}(\Omega)$ and $\mathbf{g} \in W^{m+2-1/p,p}(\Gamma)^N$ satisfy condition [39]. Then the problem (S) has a unique solution $(\mathbf{u}, \pi) \in W^{m+2,p}(\Omega)^N \times W^{m+1,p}(\Omega)/\mathbb{R}$.

Remark 28 It is possible to solve (S) under weaker assumption, for instance, if $f \in W^{-1/p}(\Omega')$, $h = 0$ and $g \in W^{-1/p,p}(\Gamma)^N$. We can prove that then $(u, \pi) \in L^p(\Omega)^N \times W^{-1,p}(\Omega)$.

The Linearized Elasticity

The equations governing the displacement $u = (u_1, u_2, u_3)$ of a three-dimensional structure subjected to an external force field f are written as (Ω is a bounded open subset of \mathbb{R}^3 and $\Gamma = \partial\Omega$)

$$\begin{aligned} -\mu\Delta u - (\lambda + \mu)\nabla(\nabla \cdot u) &= f \quad \text{in } \Omega \\ u &= 0 \quad \text{on } \Gamma_0 \end{aligned}$$

$$\sum_{j=1}^3 \sigma_{ij}(u) v_j = g_i \quad \text{on } \Gamma_1 = \Gamma - \Gamma_0$$

where $\lambda > 0$ and $\mu > 0$ are two material characteristic constants, called the Lamé coefficients, and $(v = (v_1, v_2, v_3))$

$$\begin{aligned} \sigma_{ij}(v) &= \sigma_{ji}(v) \\ &= \lambda \delta_{ij} \sum_{k=1}^3 \varepsilon_{kk}(v) + 2\mu \varepsilon_{ij}(v) \end{aligned} \quad [41]$$

$$\text{with } \varepsilon_{ij}(v) = \varepsilon_{ji}(v) = \frac{1}{2}(\partial_i v_j + \partial_j v_i)$$

where δ_{ij} denotes the Kronecker symbol, that is, $\delta_{ij} = 1$, for $i = j$ and $\delta_{ij} = 0$, for $i \neq j$. These equations describe the equilibrium of an elastic homogeneous isotropic body that cannot move along Γ_0 ; along Γ_1 , surface forces of density $g = (g_1, g_2, g_3)$ are given. The case $\Gamma_1 = \emptyset$ physically corresponds to clamped structures. The matrix with entries $\varepsilon_{ij}(u)$ is the linearized strain tensor while $\sigma_{ij}(u)$ represents the linearized stress tensor; the relationship [41] between these tensors is known as Hooke's law. We refer for example to Ciarlet and Lions (1991) and Nečas and Hlaváček (1981) (and references therein) for most of the results stated in this paragraph. The variational formulation of this problem is

$$\begin{aligned} \text{to find } u \in V \text{ such that} \\ \mathcal{A}(u, v) = L(v) \text{ for all } v \in V \end{aligned} \quad [42]$$

where the bilinear form \mathcal{A} and the linear form L are given by

$$\begin{aligned} \mathcal{A}(u, v) &= \int_{\Omega} [\lambda(\nabla \cdot u)(\nabla \cdot v) \\ &\quad + 2\mu \sum_{i,j=1}^3 \varepsilon_{ij}(u) \varepsilon_{ij}(v)](x) dx, \end{aligned} \quad [43a]$$

$$L(v) = \int_{\Omega} f(x) \cdot v(x) dx + \int_{\Gamma_1} g(\sigma) \cdot v(\sigma) d\sigma \quad [43b]$$

The functional space V is defined as

$$\begin{aligned} V &= \{v = (v_1, v_2, v_3) \in [H^1(\Omega)]^3; \\ &\quad \gamma_0 v_i = 0 \text{ on } \Gamma_0, 1 \leq i \leq 3\} \end{aligned}$$

To prove the ellipticity of \mathcal{A} , one needs the following Korn inequality: There exists a positive constant $C(\Omega)$ such that, for all $v = (v_1, v_2, v_3) \in [H^1(\Omega)]^3$, we have

$$\|v\|_{1,\Omega} \leq C(\Omega) \left[\sum_{i,j=1}^3 \|\varepsilon_{ij}(v)\|_{L^2(\Omega)}^2 + \sum_{i=1}^3 \|v_i\|_{L^2(\Omega)}^2 \right]^{1/2} \quad [44]$$

The following result holds true:

Theorem 29 Let Ω be a bounded open in \mathbb{R}^3 with a Lipschitz boundary, and let Γ_0 be a measurable subset of Γ , whose measure (with respect to the surface measure $d\Gamma(x)$) is positive. Then the mapping

$$v \mapsto \left[\sum_{i,j=1}^3 \|\varepsilon_{ij}(v)\|_{L^2(\Omega)}^2 \right]^{1/2}$$

is a norm on V , equivalent to the usual norm $\|\cdot\|_{1,\Omega}$.

As a consequence, we get:

Theorem 30 Under the above assumptions, there exists a unique $u \in V$ solving the variational problem [42]–[43]. This solution is also the unique one which minimizes the energy functional

$$\begin{aligned} E(v) &= \frac{1}{2} \int_{\Omega} \left[\lambda(\nabla \cdot v)^2 + 2\mu \sum_{i,j=1}^3 [\varepsilon_{ij}(v)]^2 \right](x) dx \\ &\quad - \left[\int_{\Omega} f(x) \cdot v(x) dx + \int_{\Gamma_1} g(\sigma) \cdot v(\sigma) d\sigma \right] \end{aligned}$$

over the space V .

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See also: Evolution Equations: Linear and Nonlinear; Γ -Convergence and Homogenization; Image Processing: Mathematics; Inequalities in Sobolev Spaces; Partial Differential Equations: Some Examples; Schrödinger Operators; Separation of Variables for Differential Equations; Viscous Incompressible Fluids: Mathematical Theory.

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Entanglement

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Introduction

Entanglement is a type of correlation between subsystems, which cannot be explained by the action of a classical random generator. It is a key notion of quantum information theory and corresponds closely to the possibility of channels which transmit quantum information, and cannot be simulated by classical channels. In this article, we consider the development of the concept, and its qualitative aspects. The quantitative aspects are treated in a separate article (*see* Entanglement Measures).

Historical Development

The first realization that quantum mechanics comes with new, and perhaps rather strange, correlations came in the famous 1935 paper by Einstein, Podolsky, and Rosen (EPR) (Einstein *et al.* 1935), in which they set up a paradox showing that the statistics of certain quantum states could not be realized by assigning wave functions to subsystems. It was in response to this paper that Schrödinger (1935), in the same year, coined the term “entanglement,” as well as its German equivalent “*Verschränkung*.” The subject lay dormant for a long time, since Bohr, in his reply, completely ignored the entanglement theme, and there was a widespread reluctance in the physics community to

consider problems of interpretation. The leaf turned slowly with Bohm's reduced model of the EPR paradox using spins rather than continuous variables, and decisively with Bell's 1964 strengthening of the paradox (Bell 1964). He showed that not only wave functions assigned to individual systems failed to describe the correlations predicted by quantum mechanics, but any set of classical parameters assigned to the subsystems. This eliminated all reference to a possibly dubious quantum ontology and all reference to the quantum formalism from the argument. Bell derived a set of inequalities from the assumption that each subsystem could be described in terms of classical variables, and that these (possibly hidden) variables would not be changed by the mere choice of a measurement for the distant correlated system. The only relation to quantum mechanics was then the simple quantum calculation showing, in certain situations, such as the state described by EPR, quantum mechanics predicted a violation of Bell's inequalities. This immediately suggested an experiment, and although it was difficult at first to find an efficient source of suitably quantum-correlated pairs of particles, the experiments that have been made since then have supported the quantum-mechanical result beyond reasonable doubt. This came too late for Einstein, whose research program in quantum mechanics had been precisely to build a “local hidden-variable theory” of the type seen in contradiction with Bell's inequality. But at least the EPR paper had finally received the response it deserved.

In Schrödinger's work, entanglement was a purely qualitative term for the strange way the subsystems

seemed to be intertwined as soon as one insisted on discussing their individual properties. After Bell's work, the favored mathematical definition of entanglement would probably have been the existence of measurements on the subsystems, such that Bell's inequality (or some generalization derived on the same assumptions) is violated. However, around 1983 another notion of (the lack of) entanglement was independently proposed by Primas (1983) and Werner (1983). According to this definition, a quantum state ρ is called unentangled if it can be written as

$$\rho = \sum_{\alpha} p_{\alpha} \rho_{\alpha}^1 \otimes \rho_{\alpha}^2 \quad [1]$$

where the ρ_{α}^i are arbitrary states of the subsystems ($i = 1, 2$), which depend on a "hidden variable" α , drawn by a classical random generator with probabilities p_{α} . Such states are now called separable, which is a bit awkward, since the notion is typically applied to systems which are widely separated. However, the term is so firmly established that it is hopeless to try to improve on it.

In any case, it was shown by Werner (1989) that there are nonseparable states, which nevertheless satisfy Bell's inequalities and all its generalizations. The next step was the observation by Popescu (1994) that entanglement could be distilled: this is a process by which some number of moderately entangled pair states is converted to a smaller number of highly entangled states, using only local quantum operations, and classical communication between the parties. For some time it seemed that this might close the gap, that is, that the failure of separability might be equivalent to "distillability" (i.e., the existence of a distillation procedure producing arbitrarily highly entangled states from many copies of the given one). However, this turned out to be false, as shown by the Horodecki family in 1998 (Horodecki *et al.* 1998), by explicitly exhibiting bound entangled, that is, nonseparable, but also not distillable states. In 2003 Oppenheim and the Horodeckis introduced a further distinction, namely whether it is possible to extract a secret key from copies of a given quantum state by local quantum operations and public classical communication (Horodecki *et al.* 2005). This task had hitherto been viewed as an application of entanglement distillation, but it turned out that secret key can be distilled from some bound entangled (but never from separable) states.

For the entanglement theory of multipartite states, that is, states on systems composed of three or more parts, between which no quantum interaction takes place, one key observation is that new entanglement properties must be expected with any increase of the

number of parties. As shown by Bennett *et al.* (1999), there are states of three parties which cannot be written in the three-party analog of [1], but are nevertheless separable for all three splits of the system into one vs. two subsystems.

The crucial advance of entanglement theory, however, lies not so much in the distinctions outlined above, but in the quantitative turn of the theory. With the discovery of the teleportation and dense coding processes (Bennett and Wiesner 1992, Bennett *et al.* 1993), entanglement changed its role from a property of counterintuitive contortedness to a resource, which is used up in teleportation and similar processes. Distillation is then seen as a method to upgrade a given source to a new source of highly entangled states suitable for this purpose, and it is not just the possibility of doing this, but the rate of this conversion, which becomes the focus of the investigation. All the tasks in which entanglement appears suggest quantitative measures of entanglement. In addition, there are many entanglement measures, which appear natural from a mathematical point of view, or are introduced simply because they can be estimated relatively easily and in turn give bounds on other entanglement measures of interest. The current situation is that there is no shortage of entanglement measures in the literature, but it is not yet clear which ones will be of interest in the long run. Some of these measures are described in Entanglement Measures.

The current state of entanglement theory is marked firstly by some long-standing open problems in the basic bipartite theory on the one hand (additivity of the entanglement of formation, the existence of NPT bound entangled states, and more recently the existence of entangled states with vanishing key rate). Secondly, there is significant effort to try to compute some of the entanglement measures, at least for simple subclasses of states. This is so difficult, because many definitions involve an optimization over operations on an asymptotically large system. Thirdly, there is a new trend in multipartite entanglement theory, namely looking specifically at entanglement in lattice structures such as spin systems of harmonic-oscillator lattices. Here one can expect very fruitful interaction with the statistical mechanics and solid-state physics in the near future.

Qualitative Entanglement Theory

Setup

Throughout this section, we will consider density operators on a Hilbert space split in some fixed way into a tensor product of a Hilbert space \mathcal{H}_A for

Alice's system and a Hilbert space \mathcal{H}_B for Bob's system, that is, $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. For simplicity, we will mostly consider finite-dimensional spaces, and if a dimension parameter $d < \infty$ appears, it is understood that $d = \dim \mathcal{H}_A = \dim \mathcal{H}_B$. By $\mathcal{B}(\mathcal{H})$ we will denote the set of bounded operators on a Hilbert space, and by $\mathcal{B}_*(\mathcal{H})$ the set of trace-class operators. We distinguish these even in the finite-dimensional case, because of their different norms. By \mathfrak{S} we will denote the state space of the combined system, that is, the set of positive elements of $\mathcal{B}_*(\mathcal{H})$ with trace 1.

For such a density operator $\rho = \rho^{AB}$ we denote by ρ^A and ρ^B the restrictions to the subsystems, defined by the partial trace over the other system, or by $\text{tr}(\rho^A F) = \text{tr}(\rho^{AB}(F \otimes \mathbb{1}))$. We denote by Θ the operation of matrix transposition, and by $\text{id} \otimes \Theta$ the partial transposition, applied only to the second tensor factor. Since transposition is not completely positive (see Channels in Quantum Information Theory) partial transposition may take positive operators to non-positive operators. The relative entropy (see Entropy and Quantitative Transversality) of two density operators ρ, σ will be used with the convention $S(\rho||\sigma) = \text{tr} \rho(\log \rho - \log \sigma)$.

Witnesses and the Criterion of Positivity of Partial Transpose

A state ρ is called separable iff it is of the form [1], and entangled otherwise. The set of separable states \mathfrak{C} is a convex subset of the set \mathfrak{S} of all states. Its extreme points are obvious from the representation [1], namely the pure product states $\rho = |\phi_A \otimes \phi_B\rangle\langle\phi_A \otimes \phi_B|$. Since \mathfrak{C} , like \mathfrak{S} , is a convex set in $(d^4 - 1)$ dimensions, Caratheodory's theorem asserts that the sum can be taken to be a decomposition into d^4 such terms. For a given ρ , deciding whether it is separable or entangled, hence, involves a nonlinear search problem in roughly $4d^5$ real parameters, namely the vector components of the ϕ_A, ϕ_B appearing in the sum.

Dually, the convex set \mathfrak{C} can be described by a set of linear inequalities. Here is a simple way of generating such inequalities: let $T: \mathcal{B}_*(\mathcal{H}_B) \rightarrow \mathcal{B}(\mathcal{H}_A)$ be a positive linear map, that is, a map taking positive matrices to positive matrices. Then for $\rho_A, \rho_B \geq 0$ the expression $\text{tr}(\rho_A T(\rho_B))$ is positive. It is also bilinear, so we can find a Hermitian operator $T^\natural \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$ such that

$$\text{tr}(\rho_A T(\rho_B)) = \text{tr}((\rho_A \otimes \rho_B) T^\natural)$$

Since the left-hand side is positive, we see by taking convex combinations that $\text{tr}(\rho T^\natural) \geq 0$ for all separable states ρ . Hence, if we find a state with a negative expectation of T^\natural , we can be sure it is entangled.

Therefore, such operators T^\natural are called entanglement witnesses. This is often a useful criterion, especially when one has some additional information about the state, allowing for an intelligent choice of witness. It is known from the theory of ordered vector spaces and their tensor products that the set of witnesses constructed above is complete. Hence, in principle, checking all such witnesses provides a necessary and sufficient criterion for entanglement. However, in practice this remains a difficult task, because the extreme points of the set of positive maps are only known for some low dimensions.

By restricting T to completely positive maps, we get a useful necessary criterion. It can be seen that it is equivalent to

$$(\text{id} \otimes \Theta)(\rho) \geq 0$$

that is, to the positivity of the partial transpose (PPT). States with this property are called "PPT states" in current jargon.

Pure States, Purification

For pure states, that is, for the extreme points of \mathfrak{S} , separability is trivial to decide: since for pure states the sum [1] can only be a single term, a pure state is separable iff it factorizes.

A useful observation is that, for pure states $\rho = |\Phi\rangle\langle\Phi|$, all information about entanglement is contained in the spectrum of the reduced states. Consider a vector $\Phi \in \mathcal{H}_A \otimes \mathcal{H}_B$ of the form

$$\Phi = \sum_{\alpha} \sqrt{r_{\alpha}} \phi_{\alpha}^A \otimes \phi_{\alpha}^B \quad [2]$$

where $\phi_{\alpha}^A \in \mathcal{H}_A$ and $\phi_{\alpha}^B \in \mathcal{H}_B$ are orthonormal systems, $r_{\alpha} > 0$, and $\sum_{\alpha} r_{\alpha} = 1$. Then it is easy to check that $\rho^A = \sum_{\alpha} r_{\alpha} |\phi_{\alpha}^A\rangle\langle\phi_{\alpha}^A|$ is the spectral resolution of the restriction. Conversely, by diagonalizing the restriction of a general unit vector Φ , we find a biorthogonal decomposition of the form [2], also known as the Schmidt decomposition. The Schmidt spectrum $\{r_1, \dots, r_d\}$ hence classifies vectors up to local basis changes in \mathcal{H}_A and \mathcal{H}_B .

Since any ρ^A can appear in this construction, we see that any mixed state can be considered as the restriction of a pure state, which is essentially unique, namely up to the choice of basis in the purifying system B, and up to perhaps adding or deleting some irrelevant dimensions in \mathcal{H}_B . The resulting vector Φ is known as the purification of ρ_A .

The extreme cases of [2] are pure product states on the one hand, and vectors, for which $\rho^A = \mathbb{1}/d$ is the totally chaotic state. These are known as maximally entangled and embody, in the most extreme way, the observation that in quantum

mechanics, as opposed to classical probability, the restriction of a pure state may be mixed.

Let us fix a maximally entangled vector Ω , and the matching Schmidt bases, so that

$$\Omega = \frac{1}{\sqrt{d}} \sum_k |kk\rangle \quad [3]$$

where we have used the simplified ket notation, in which only the basis label is written. Then, an arbitrary vector can be written as $\Phi = (X \otimes 1)\Omega = (1 \otimes X^T)\Omega$, where X^T denotes the matrix transpose of X . Clearly, this vector is again maximally entangled iff X is unitary. Hence, the set of maximally entangled vectors is a single orbit under unilateral unitary transformations, and we even have the choice to which side we apply the unitaries.

Teleportation

Suppose we have an orthonormal basis of maximally entangled vectors $\Phi_\alpha \in \mathcal{H}_A \otimes \mathcal{H}_B$. By the remarks above, this is equivalent to choosing unitaries $U_\alpha, \alpha = 1, \dots, d^2$ such that $\Phi_\alpha = (U_\alpha \otimes 1)\Omega$, and $\text{tr}(U_\alpha^* U_\beta) = d\delta_{\alpha\beta}$. For example, a finite Weyl system constitutes such a system of unitaries, which shows that we can find realizations in any dimension d .

Suppose that Alice and Bob each own part of a system prepared in the state Ω then they can transmit perfectly the state of a d -dimensional system, using only classical communication. Classical communication by itself would never suffice to transmit quantum information, and the entangled resource Ω by itself does not allow the transmission of any signal. But the combination of these resources does the trick: Alice measures the observable associated with the basis Φ_α on the combined system formed by the unknown input and her part of the entangled pair. The result α is then transmitted to Bob, who performs a U_α -rotation on his part of the entangled pair, producing the output state of the teleportation. One can show by direct calculation that this is exactly equal to the input state.

Note that the resource Ω is destroyed in this process, so that for every transmission we need a fresh entangled pair. Less than maximally entangled states instead of Ω lead to less-than-perfect transmission, which can be extended to quantitative relations between entanglement and channel capacity.

Special Systems

Qubits

For qubit pairs, there is a special basis of maximally entangled vectors, which has some amazing

properties. It consists of the vectors $\Phi_0 = \Omega$, and $\Phi_k = i(\sigma_k \otimes 1)\Omega$, where $\sigma_k, k = 1, 2, 3$, denotes the Pauli matrices. Then a vector is maximally entangled iff its components are real in this basis, up to a common phase. A unitary matrix of determinant 1 factorizes into $U_1 \otimes U_2$ iff its matrix elements are real, up to a common phase.

For qubit pairs, and also for dimensions $2 \otimes 3$, the partial transposition criterion for entanglement is necessary and sufficient, as shown by Woronowicz and the Horodecki family.

Orthogonally Invariant States

A state ρ on $\mathbb{C}^d \otimes \mathbb{C}^d$ is called orthogonally invariant if, for any orthogonal matrix U (with respect to some fixed product basis) $[\rho, U \otimes U] = 0$. This leaves a three-dimensional space of operators, spanned by the identity, the permutation $F = \sum_{i,j} |ij\rangle\langle ji|$, and its partial transpose $\hat{F} = \sum_{i,j} |ii\rangle\langle jj|$, which is d times the projection onto the maximally entangled vector Ω . Figure 1 shows the plane of Hermitian operators ρ with the described symmetry and $\text{tr} \rho = 1$. Convenient coordinates are $\text{tr} \rho F$ and $\text{tr} \rho \hat{F}$. Note that these are defined for any density operator, and are also invariant under the “twirl” operation $\rho \mapsto \int dU (U \otimes U) \rho (U \otimes U)^*$, using the Haar measure dU , which projects onto the orthogonally invariant states. Hence, the diagram provides a section as well as a projection of the state space. The intersection of the positive operators with those having positive partial transpose is the set of PPT states, which in this case coincides with the separable states. The thin lines correspond to states of higher symmetry, namely on the one hand the “isotropic states” commuting with $U \otimes \bar{U}$, with \bar{U} the complex conjugate of U , and the “Werner states” commuting with all unitaries $U \otimes U$. Their intersection point is the normalized trace.

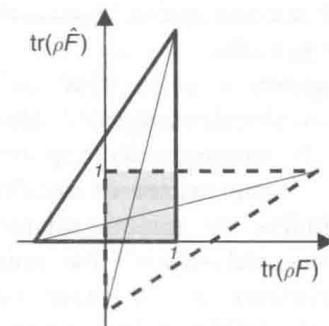


Figure 1 The plane of orthogonally invariant unit trace Hermitian operators of a $3 \otimes 3$ -system. The upright triangle gives the positive operators, and the dashed one those with positive partial transpose. The shaded area gives the PPT states.

Gaussians

In general, the entanglement in systems with infinite-dimensional Hilbert spaces is more difficult to analyze. However, if the system is characterized by variables satisfying canonical commutation relations, like positions and momenta, or the components of the free quantum electromagnetic field, there is a special class of states, which is again characterized by low-dimensional matrices. This allows the discussion of entanglement questions, in a way largely parallel to the finite-dimensional theory.

Let R_1, \dots, R_{2f} denote the canonical operators, where f is the number of degrees of freedom. The commutation relations can be summarized as $i[R_\mu, R_\nu] = \sigma_{\mu\nu} 1$, where σ is the symplectic matrix. Operators R_μ have a common set of analytic vectors, and generate the unitary Weyl operators $W(a) = \exp(ia^\mu R_\mu)$, which describe the phase space displacements. Gaussian states are those making $a \mapsto \text{tr } \rho W(a)$ a Gaussian function or, equivalently, those with Gaussian Wigner function. Up to a global displacement, they are completely characterized by the covariance matrix

$$\gamma_{\mu\nu} = \text{tr } \rho(R_\mu R_\nu + R_\nu R_\mu) \quad [4]$$

The only constraint for a real symmetric matrix to be a covariance matrix of a quantum state is that $\gamma + i\sigma$ is a positive semidefinite matrix, which is a version of the uncertainty relations.

Now for entanglement theory, we take some of the degrees of freedom as Alice's and some as Bob's. Separability can be characterized in terms of γ , namely by the condition that $\gamma \geq \gamma'$, where γ' is the covariance matrix of a Gaussian product state. Similarly, partial transposition can be implemented as an operation on covariance matrices, which allows a simple verification of the PPT condition. It turns out that as long as one partner has only a single degree of freedom, the PPT condition is necessary and sufficient for separability, but this fails for larger systems.

The pure Gaussian states allow a normal form with respect to local symplectic transformations analogous to the Schmidt decomposition. For the minimal case of one degree of freedom on either side, one obtains a one-parameter family of "two mode squeezed states." Its limit for infinite squeezing parameter is the state used by EPR (Einstein *et al.* 1935), which, however, makes rigorous mathematical sense only as a singular state, that is, a linear functional on $\mathcal{B}(\mathcal{H})$, which can no longer be represented as the trace with a density operator.

Multipartite Stars

A key feature of entanglement in a multipartite system is usually referred to as "monogamy": when Alice shares a highly entangled state with Bob, her system cannot also be highly entangled with Bill. More formally, suppose that a multipartite state for systems A, B_1, \dots, B_n is given, such that the restriction to each pair AB_k is the same bipartite state ρ . Then as n becomes larger, the existence of such a star-shaped extension constrains ρ to become less and less entangled. In fact, as $n \rightarrow \infty$, this condition is equivalent to the separability of ρ .

Open Problems

Recall from the introduction the following chain of inclusions:

$$\begin{aligned} \text{separable states} &\subset \text{states with vanishing key rate} \\ &\subset \text{PPT state} \\ &\subset \text{undistillable states} \\ &\subset \text{all states} \end{aligned}$$

The second and fourth inclusions are strict, but for the first and third one might have equality, for all we know. Especially for the third inclusion, this is a long-standing problem.

Finally, we would like to point out that qualitative and conceptual aspects of entanglement are surveyed by Bub (2001), Popescu and Rohrlich (1998), and Horodecki *et al.* (2001). For quantitative aspects see Entanglement Measures.

See also: Capacities Enhanced by Entanglement; Capacity for Quantum Information; Channels in Quantum Information Theory; Entanglement Measures; Entropy and Quantitative Transversality.

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Entanglement Measures

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Introduction

Entanglement, or quantum correlation, is one of the central concepts in quantum information theory. Its theory can be roughly separated into three parts. The first is *qualitative*, that is, it addresses the question “Is this state entangled or not?” The second, *comparative* part asks “Is this state more entangled than that state?” and finally the *quantitative* theory asks “How entangled is this state?” and gives its answers in the form of entanglement measures assigning a number to every state. Quantitative questions come up naturally whenever entanglement is used as a resource for tasks of quantum information processing. For example, entangled states are in a way the fuel for the processes of teleportation and dense coding: in each transmission step a maximally entangled pair system is required, and cannot be used for a further transmission. The process also works with less than maximally entangled states, but then it also becomes less efficient. Since entangled states created in the laboratory typically have imperfections, it becomes important to understand the rates at which imperfectly entangled states may be distilled to maximally entangled ones, and this rate is a direct measure of the usefulness of the given state for many purposes. The quantitative, task related turn is a new development in the study of the foundations of quantum mechanics. It has been imported from classical information theory, where this way of thinking has been standard for a long time. The combination makes the particular flavor of quantum information theory.

In this article we consider the comparative and quantitative aspects of entanglement. The historical aspects and qualitative theory are treated in a separate article (*see* Entanglement), to which we refer for basic notions and notations. The example of teleportation suggests close links between quantitative entanglement theory and the theory of capacity Bennett *et al.* (1996), which is the transfer rate of quantum information through a given channel. These connections are described in Quantum Channels: Classical Capacity.

We follow the notations of the basic article on entanglement (*see* Entanglement). In particular, Θ denotes the transpose operation, and $(\text{id} \otimes \Theta)$ the partial transpose. A state is called “PPT” if its partial transpose is positive. The two physicists operating the laboratories in which the two parts of a bipartite system are kept are called Alice and Bob, as usual. The restriction of a state ρ to Alice’s subsystem is denoted by ρ^A .

Comparative Entanglement and Protocols

Protocols

In this section we introduce relations of the kind “state ρ_1 is more entangled than ρ_2 .” We take this to mean that ρ_2 can be obtained by applying to ρ_1 some operations which “cannot create entanglement.” The definition of a class of operations of which this can be claimed then defines the comparison. It turns out that there are different choices for the class of such operations, depending on the resources available for the transformation steps. The class of operations is usually referred to as a *protocol*.

Certainly local operations performed separately by Alice and Bob cannot increase entanglement. Alice and Bob might have to make some choices, and even if they make these according to a

prearranged scheme, by using a shared table of random numbers, entanglement will not be generated. In this restrictive protocol, which we abbreviate by LO, for “local operations,” no communication is allowed. It is clear that by just discarding the initial state, and preparing a new one, based on the random instruction allows Alice and Bob to make any separable state, so these states come out as the “least entangled” ones for this and any richer protocol.

Next we might allow classical communication from Alice to Bob. That is, Bob’s decision to perform some operation in his laboratory is allowed to depend on measuring results obtained by Alice in an earlier stage. Of course, Alice is not allowed to send quantum systems, since in this case she might just send a particle entangled to one of her own, and any state could be generated. This protocol is referred to as “local operations and one-way classical communication” (LOWC). Obviously, we might also allow Bob to talk back, arriving at “local operations and classical communication” (LOCC). This is the protocol underlying most of the work in entanglement theory.

The drawback of the LOCC protocol is that its operations are extremely difficult to characterize: an LOCC operation can take many rounds, and there is no way to simplify a general operation to some kind of standard form. This is the main reason why other protocols have been considered. For example, it is obvious that an LOCC operation can be written as a sum of tensor products of local operations, in a form reminiscent of the definition of separability. However, such “separable superoperators” may fall outside LOCC. Another property easily checked for all LOCC operations is that PPT states go into PPT states. The protocol “PPT-preserving operations” (PPTP) can also be characterized as the set of channels T for which $(\text{id} \otimes \Theta)T(\text{id} \otimes \Theta)$ is positive (although not necessarily completely positive). This condition is relatively easy to handle mathematically, so that the best way to show that some ρ_1 cannot be converted to ρ_2 by LOCC is often to show that this transition is impossible under PPTP. The drawback of the PPTP protocol is that it may create some entanglement after all, namely arbitrary PPT states. So it properly belongs to a modified entanglement theory in which separability is replaced by the PPT condition.

Converting Pure States and Majorization

The entanglement ordering is exactly known for pure states due to a famous theorem by Nielsen (1999): a pure state ρ_1 is *more entangled* than a pure

state ρ_2 under the LOCC protocol iff the restriction ρ_1^A is *more mixed* than the restriction ρ_2^A in the sense of majorization of spectra (i.e., for every k the sum of the k largest eigenvalues of ρ_1^A is less than the corresponding sum for ρ_2^A). Equivalently, there is a doubly stochastic channel (completely positive linear map preserving both the identity and the trace functional) taking ρ_2^A to ρ_1^A .

An interesting aspect of this theory is the phenomenon of *catalysis*: It may happen that although ρ_1 cannot be converted by LOCC to ρ_2 , $\rho_1 \otimes \sigma$ can be converted to $\rho_2 \otimes \sigma$. The “catalyst” σ is a resource borrowed at the beginning of the transformation, and is returned unchanged afterwards. The order relation allowing such catalysts is yet to be fully characterized.

Asymptotic Conversion

In many applications we are not interested in exact conversion of one state to another, but are quite satisfied if the transformation can be done with a small controlled error. In particular, when we ask for the *achievable conversion rate* between many copies of the states involved, we allow small errors, but require the errors to go to zero. Given any protocol, and states ρ_1, ρ_2 , we say that ρ_1 can be converted to ρ_2 with rate r if, for all sufficiently large n , there is a channel of the protocol, which takes n copies of ρ_1 , that is, the state $\rho_1^{\otimes n}$, to a state ρ' which approximates roughly $m \approx rn$ copies of ρ_2 , in the sense that $m \geq rn$, and the trace norm $\|\rho' - \rho_2^{\otimes m}\|$ goes to zero.

Of course, one is usually interested in the supremum of the achievable conversion rates, which we call simply the maximal conversion rate. In particular, when ρ_2 is the maximally entangled pure state of a qubit pair (usually called the “singlet”), the maximal rate is called the *distillable entanglement* $E_D(\rho_1)$. In the other direction, when ρ_1 is the singlet, we call the inverse of the maximal conversion rate the *entanglement cost* $E_C(\rho_2)$. These are two of the key entanglement measures to be discussed below.

In general, $E_D(\rho) < E_C(\rho)$, so the asymptotic conversion between different states is usually not reversible. However, this is the case for pure states, and one finds

$$E_D(\rho) = E_C(\rho) = S(\rho^A) \quad [1]$$

where $S(\rho) = -\text{tr} \rho \log_2(\rho)$ denotes the von Neumann entropy (see Entropy and Quantitative Transversality) based on the binary logarithm.

Since one can do the conversion between different pure states via singlets, it is clear that the maximal conversion rate from a pure state ρ_1 to a pure state ρ_2

equals $S(\rho_1^A)/S(\rho_2^A)$. Hence, in contrast to the ordering given by Nielsen's theorem, all pure states are interconvertible, and the ordering is described by a single number. For this simplification, the allowance of small errors is crucial. Without asymptotically small but nonzero errors, it would also be impossible to obtain singlets from any generic mixed state.

Entanglement Measures

Properties of Interest

We now consider more systematically functions $E: \mathcal{S} \rightarrow \mathbb{R}$ defined on the states spaces of arbitrary bipartite quantum systems. When can we regard this as a measure of entanglement? The minimal requirements are that $E(\rho) \geq 0$ for all ρ , and $E(\rho) = 0$ for separable states. Since the choice of local bases should be irrelevant, we will require $E((U_A \otimes U_B)\rho(U_A \otimes U_B)^*) = E(\rho)$ for unitaries U_A, U_B . We also *normalize* all entanglement measures so that $E(\sigma) = 1$, when σ is the maximally entangled state of a pair of qubits. Beyond that, consider the following:

1. V (*Convexity* $E(\sum_{\alpha} p_{\alpha} \rho_{\alpha}) \leq \sum_{\alpha} p_{\alpha} E(\rho_{\alpha})$) Starting from any E , possibly defined only on a subset containing the pure states, we can enforce this property by taking the *convex hull* (or "roof") $\text{co}E$, defined as the largest convex function, which is $\leq E$ wherever it is defined.
2. M (*Monotonicity*) Suppose that some LOCC protocol applied to ρ returns some classical parameter α with probability p_{α} , and in that case a bipartite state ρ_{α} . Then $\sum_{\alpha} p_{\alpha} E(\rho_{\alpha}) \leq E(\rho)$.
3. A^{-} (*Subadditivity* $E(\rho_1 \otimes \rho_2) \leq E(\rho_1) + E(\rho_2)$) In this and the following, the tensor products of bipartite states are to be reordered from $A_1 B_1 A_2 B_2$ to $(A_1 A_2)(B_1 B_2)$, so the separation into Alice's and Bob's subsystems is respected.
4. A^{+} (*Superadditivity* $E(\rho_1 \otimes \rho_2) \geq E(\rho_1) + E(\rho_2)$)
5. A^{++} (*Strong superadditivity* $E(\rho_{12}) \geq E(\rho_1) + E(\rho_2)$) Here ρ_i denotes the restriction of a general state ρ_{12} to the i th subsystem.
6. A^{∞} (*Weak additivity* $E(\rho^{\otimes n}) = nE(\rho)$) This can be enforced by *regularization*, going from E to

$$E^{\infty}(\rho) = \lim_{n \rightarrow \infty} \frac{1}{n} E(\rho^{\otimes n})$$

Note that this is implied by *additivity*, which is the conjunction of A^{+} and A^{-} .

7. C (*Continuity*) Here it is crucial to postulate the right kind of dimensional dependence. A good choice is to demand that $|E(\rho_1) - E(\rho_2)| \leq \log df(\|\rho_1 - \rho_2\|)$, where f is some function with $\lim_{t \rightarrow 0} f(t) = 0$.

8. L (*Lockability*) A property related to, but not equal to, discontinuity: a measure is called lockable, if the loss (i.e., the tracing out) of a single qubit by Alice or Bob can make $E(\rho)$ drop by an arbitrarily large amount.

The Collection of Entanglement Measures

The following are the main entanglement measures discussed in the literature. Note that all measures defined by conversion rates in principle depend on the protocol used. Unless otherwise stated, we will only consider LOCC. For every function we list in brackets the properties which are known.

1. E_F (*Entanglement of formation* $[V, M, A^{-}, C, L]$) This is defined as the convex hull of the entanglement of pure states given by eqn [1]. For qubit pairs, there is a closed formula due to Wootters (1998), orthogonally invariant states (Vollbrecht and Werner 2001) (see 00510), and permutation symmetric 2-mode Gaussians. One of the big open questions is whether E_F is additive. This is equivalent to E_F satisfying A^{++} , and also to the additivity of Holevo's χ -capacity of quantum channels (see Quantum Channels: Classical Capacity).
2. E_C (*Entanglement cost* $[V, M, A^{-}, A^{\infty}, C, L]$) This was already defined in the section "Asymptotic conversion." It has been shown to be equal to the regularization of E_F , that is, $E_C = E_F^{\infty}$. If E_F would turn out to be additive, we would thus have $E_C = E_F$.
3. E_D (*Distillable entanglement* $[M, A^{++}, A^{\infty}]$) Again, see the section "Asymptotic conversion." This is one of the important measures from the practical point of view, but notoriously difficult to compute explicitly. Convexity of E_D is an open problem related to the existence of bound entangled, but not PPT states.
4. E_{\rightarrow} (*One-way distillable entanglement* $[M, A^{++}, A^{\infty}]$) Same as E_D , but restricting to the LOWC protocol. Obviously, $E_{\rightarrow}(\rho) \leq E_D(\rho)$. There are examples of proper inequality " $<$ " (Bennett *et al.* 1996). E_{\rightarrow} is more directly linked to quantum capacity than E_D , which in turn corresponds to the quantum capacity, allowing classical backwards communication as a resource.
5. E_N (*Logarithmic negativity* $[M, A^{-}, A^{+}, L]$) This is a quantitative companion of the PPT criterion: one sets $E_N(\rho) = \log_2 \|(\text{id} \otimes \Theta)(\rho)\|$, where the norm is the trace norm. For PPT states, ρ this is equal to the trace, and $E_N(\rho) = 0$. If the partial transpose has negative eigenvalues, the sum of their absolute values is >1 , and $E_N(\rho) > 0$. E_N is an easily computed upper bound to E_D , but gives the wrong value for nonmaximally entangled pure states.

6. E_R (Relative entropy of entanglement [V,M,A⁻]) This measure (Vedral *et al.* 1997) is motivated geometrically: it is simply the relative entropy distance of ρ to the separable subset: $E_R(\rho) = \inf_{\sigma} S(\rho||\sigma)$, where σ ranges over all separable states. E_R is an upper bound to E_D . However, it can be improved by taking the distance to the PPT states rather than the separable states, and by combining with E_N , in the following way:
7. E_B (The Rains bound [V,M,A⁻,C]) Following Rains (2001), we set

$$E_B(\rho) = \inf_{\sigma} (S(\rho||\sigma) + E_N(\sigma))$$

where the infimum is over all states σ . This is still an upper bound to E_D , although clearly smaller than both E_R (take only separable σ) and E_N (take $\sigma = \rho$). No example of $E_D(\rho) < E_R(\rho)$ is known, but any bound entangled non-PPT state would be such an example.

8. E_S (Squashed entanglement [V,M,A⁻,A⁺⁺,C,L]) This measure, introduced by Christandl and Winter (2004), amazingly has all the good properties, but is as difficult to compute as any of the other measures. $E_S(\rho^{AB})$ is the infimum over the entropy combination

$$S(\rho^{AC}) + S(\rho^{BC}) - S(\rho^{ABC}) - S(\rho^C)$$

over all extensions ρ^{ABC} of the given state ρ^{AB} to a system enlarged by a part C, where the density operators in the above expression are the restrictions of ρ^{ABC} to the subsystems indicated.

9. E_K (Key rate [V,M,A⁻]) The bit rate at which secret key can be generated is certainly larger than E_D , since distillation is one way to do it. It is, in general, strictly larger, since there are undistillable states with positive key rate.
10. E_C (Concurrence [V]) This measure was originally only defined for qubit pairs, as a step in Wootters's (1998) formula for E_F in this case. It has an extension to arbitrary dimensions (Rungta *et al.* 2001), namely the convex hull of

the function $c(|\psi\rangle\langle\psi|) = \sqrt{2(1 - \text{tr}(\rho^2))}$, where $\rho = |\psi\rangle\langle\psi|^A$ is the reduced density operator. Both upper and lower bounds exist in the literature. The main interest in this measure stems from the fact that it has interesting extensions to the multipartite case.

To conclude, we would like to point out that many of the themes discussed in this article were set by Bennett *et al.* (1996); their article is worth reading even today. Good review articles covering entanglement measures, with more complete references, are Plenio and Virmani (2005), Bruß (2002), and Donald *et al.* (2002).

See also: Entanglement; Entropy and Quantitative Transversality; Quantum Channels: Classical Capacity.

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Entropy and Quantitative Transversality

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Introduction

A mathematical law for a physical phenomenon, describing the variation of a value $y \in \mathbb{R}$ in terms of parameters $x_i \in \mathbb{R}, i \in \{1, \dots, n\}$, is usually given:

1. in the simplest cases (and hence in exceptional cases), by an explicit functional equation $y = F(x_1, \dots, x_n)$, or
2. by an implicit equation $G(y, x_1, \dots, x_n) = 0$, or
3. more generally, by a partial differentiable equation,

$$H\left(y, \frac{\partial^{\alpha_1} y}{\partial x_{i_1} \dots \partial x_{i_{\alpha_1}}}, \dots, \frac{\partial^{\alpha_k} y}{\partial x_{j_1} \dots \partial x_{j_{\alpha_k}}}, x_1, \dots, x_n\right) = 0 + \text{initial values}$$

In the first case, the exact equation $y = F(x_1, \dots, x_n)$ fully describes the behavior of y as (x_1, \dots, x_n) vary, but in practice this information is too substantive: using the Taylor formula, knowledge of the value y^0 at some point (x_1^0, \dots, x_n^0) and of the value of

$$\nabla F_{(x_1^0, \dots, x_n^0)} = \left(\frac{\partial F}{\partial x_1}, \dots, \frac{\partial F}{\partial x_n} \right) (x_1^0, \dots, x_n^0)$$

is enough to predict, with controlled accuracy, by linear approximation, the behavior of y for parameters (x_1, \dots, x_n) close to (x_1^0, \dots, x_n^0) .

In the case (2), both the parameters (x_1, \dots, x_n) and the value y belong to the set $M = \{(y, x_1, \dots, x_n) \in \mathbb{R}^{n+1}; G(y, x_1, \dots, x_n) = 0\}$, and we would like to know whether or not this set may be (at least locally around one of its point $(y^0, x_1^0, \dots, x_n^0)$) a graph of some function $(x_1, \dots, x_n) \mapsto y = F(x_1, \dots, x_n)$, as in the case (1). Using the implicit function theorem, we may try to reduce our equation to the explicit equation of (1), and then perform a linear approximation involving $\nabla F_{(x_1^0, \dots, x_n^0)}$. Assuming that *a priori* we know a value y^0 such that for $(x_1^0, \dots, x_n^0), (y^0, x_1^0, \dots, x_n^0) \in M$, this reduction is possible, locally around $(y^0, x_1^0, \dots, x_n^0)$, under the condition that

$$\frac{\partial G}{\partial y}(y^0, x_1^0, \dots, x_n^0) \neq 0$$

In this situation

$$\nabla F_{(x_1^0, \dots, x_n^0)} = - \left(\frac{\partial G}{\partial x_1}, \dots, \frac{\partial G}{\partial x_n} \right) \times (y^0, x_1^0, \dots, x_n^0) / \frac{\partial G}{\partial y}(y^0, x_1^0, \dots, x_n^0)$$

Now, as it is normally the case, when they come from observation, the variables x_1, \dots, x_n are known with an estimate and one sees that the larger

$$\left| \left(\frac{\partial G}{\partial x_1}, \dots, \frac{\partial G}{\partial x_n} \right) (y^0, x_1^0, \dots, x_n^0) / \frac{\partial G}{\partial y}(y^0, x_1^0, \dots, x_n^0) \right|$$

is, the worse the estimate on y near y^0 .

Furthermore, assuming that M is locally a graph of a function $(x_1, \dots, x_n) \mapsto y = F(x_1, \dots, x_n)$, for a given (x_1, \dots, x_n) , the exact expression of $y = F(x_1, \dots, x_n)$ and consequently the exact value of $\nabla F_{(x_1, \dots, x_n)}$ is not possible to obtain; we have to approach it using an algorithm (classically the Newton algorithm), and closer

$$\frac{\partial G}{\partial y}(y^0, x_1^0, \dots, x_n^0)$$

is to 0, the more such an algorithm is unstable.

Finally, in the case (3), skipping technical details, we encounter the same type of difficulties: we have to avoid small values for some gradient functions at a given point, in order to obtain, locally at some point (x_1^0, \dots, x_n^0) , in a stable way, reliable information on y in terms of (x_1, \dots, x_n) .

To sum up, the prediction of a physical phenomenon by a mathematical law greatly depends not only on the noncancellation of some gradient functions, but, as we deal with approximations and algorithms, on how different those gradient functions are from zero.

This principle, of course, extends directly to applied problems (see the last of our examples in the final section): being close to singular values essentially means that the control (e.g., of the positions of some device by a manipulator) is poor.

The geometric counterpart of this analytic phenomenon is called "transversality," the condition for some function G to have a nonzero partial derivative

$$\frac{\partial G}{\partial y}(y^0, x_1^0, \dots, x_n^0)$$

is equivalent to the condition

$$\nabla G_{(y^0, x_1^0, \dots, x_n^0)} \oplus \text{O}x_1 \dots x_n = \mathbb{R}^{n+1}$$

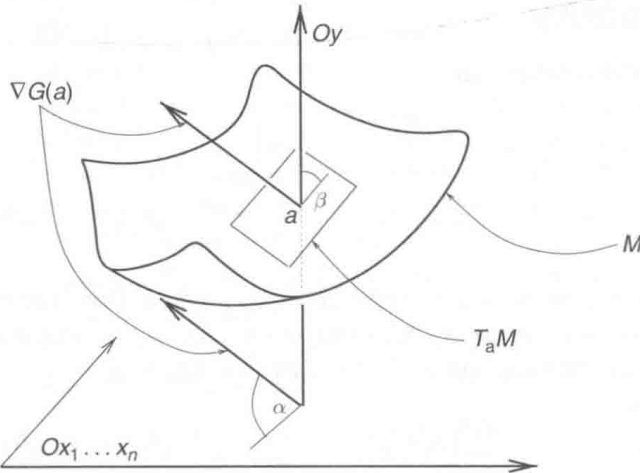


Figure 1 Transversality of the manifold M and Oy .

or to the condition

$$T_{(y^0, x_1^0, \dots, x_n^0)} M \oplus Oy = \mathbb{R}^{n+1}$$

where $T_a M$ is the tangent space of M at $a \in M$.

We say that $\nabla G_{(y^0, x_1^0, \dots, x_n^0)}$ is transverse to the space of parameters $Ox_1 \dots Ox_n$ at $(y^0, x_1^0, \dots, x_n^0)$, or that M is transverse to Oy at $(y^0, x_1^0, \dots, x_n^0)$.

For some quantity $\epsilon > 0$, the condition that

$$\left| \left(\frac{\partial G}{\partial x_1}, \dots, \frac{\partial G}{\partial x_n} \right) (y^0, x_1^0, \dots, x_n^0) / \frac{\partial G}{\partial y} (y^0, x_1^0, \dots, x_n^0) \right| \geq \frac{1}{\epsilon}$$

means that the angle $\alpha = (\nabla G_{(y^0, x_1^0, \dots, x_n^0)}, Ox_1 \dots Ox_n)$ or the angle $\beta = (T_{(y^0, x_1^0, \dots, x_n^0)} M, Oy)$ is smaller than ϵ (see Figure 1).

Our purpose in the sequel is to indicate how we can quantify the situations described above (the defect of transversality), in order to generically or almost generically avoid them with quantified accuracy.

Quantifying Transversality

Given two submanifolds M and N of the Euclidean space \mathbb{R}^n , we can measure the transversality defect of (M, N) at $x \in \mathbb{R}^n$ with a differential criterion, both analytical and geometric.

Let us first introduce some notations. For a given linear map $L: \mathbb{R}^n \rightarrow \mathbb{R}^p$, the image by L of the unit ball of \mathbb{R}^n is an r -dimensional ellipsoid in \mathbb{R}^p with semi-axes denoted as $l_1(L) \geq \dots \geq l_r(L)$, where r is the rank of L . For $r < p$, we denote $l_{r+1}(L) = 0, \dots, l_p(L) = 0$.

Now, let $x \in M \cap N$; let $\pi: \mathbb{R}^n \rightarrow T_x N^\perp$ be the projection onto the orthogonal space of $T_x N$, $p = n - \dim(N)$ and $\pi|_M$ the restriction of π to M .

Definitions

We say that (M, N) is transverse at x , and we denote it by $M \pitchfork_x N$, if and only if $\pi|_M$ is a submersion at x , that is, $D\pi|_{M(x)}: T_x M \rightarrow T_x N^\perp$ is onto.

For a given $\Lambda = (\epsilon_1, \dots, \epsilon_p)$, $\epsilon_1 \geq \dots \geq \epsilon_p$, we say that (M, N) is Λ -nontransverse at x , and we denote it by $M \not\pitchfork_x^\Lambda N$, if and only if $l_i(D\pi|_{M(x)}) \leq \epsilon_i, \forall i \in \{1, \dots, p\}$.

With these notations, we have: $M \not\pitchfork_x N$ (i.e., (M, N) nontransverse at x) if and only if $x \notin M \cap N$ or $M \not\pitchfork_x^\Lambda N$, for some Λ with $\epsilon_p = 0$, and the more (M, N) is Λ -nontransverse, with Λ close to $(\epsilon_1, \dots, \epsilon_{p-1}, 0)$, the less the manifolds M and N seem transverse at $x \in M \cap N$ (see Figure 2).

The final step in our formalism to give a convenient quantitative approach of transversality is the following: let X, Y be two (real) Riemannian manifolds, $f: X \rightarrow Y$ a (smooth) mapping, $N \subset Y$ a submanifold of Y with codimension p in N , $y \in N$, and $\Phi: \mathcal{O} \rightarrow \mathbb{R}^p$ a submersion, where \mathcal{O} is an open neighborhood of x in Y , such that $\Phi^{-1}(\{0\}) = N \cap \mathcal{O}$. Then we say that (f, N) is transverse at x , and we denote it by $f \pitchfork_x N$, if and only if $f \circ \Phi$ is submersive in x .

For a given $\Lambda = (\epsilon_1, \dots, \epsilon_p)$, $\epsilon_1 \geq \dots \geq \epsilon_p$, we say that (f, N) is (Φ, Λ) -nontransverse at x , and we denote it by $f \not\pitchfork_x^{(\Phi, \Lambda)} N$, if and only if $l_i(D[f \circ \Phi]_{(x)}) \leq \epsilon_i, \forall i \in \{1, \dots, p\}$.

Clearly, we recognize the definition of transversality and of Λ -nontransversality of two submanifolds M, N of \mathbb{R}^n by letting $f: M \rightarrow \mathbb{R}^n$ be the inclusion and $\Phi = \pi|_M$ (for more details on transversality and stability, see, e.g., Golubitski and Guillemin (1973)).

With the definitions and notations above, our general problem may be posed as follows:

For a C^k -regular ($k \in \mathbb{N} \cup \{\infty\}$) mapping $f: \mathbb{R}^n \rightarrow \mathbb{R}^p$ and a given $\Lambda = (\epsilon_1, \dots, \epsilon_p)$, how large is the set $\Delta(f, B_r, \Lambda) = f(\Sigma(f, B_r, \Lambda))$, where $\Sigma(f, B_r, \Lambda) = \{x \in B_r \subset \mathbb{R}^n; l_i(Df_{(x)}) \leq \epsilon_i, \forall i \in \{1, \dots, p\}\}$ and B_r is a ball of radius r in \mathbb{R}^n ?

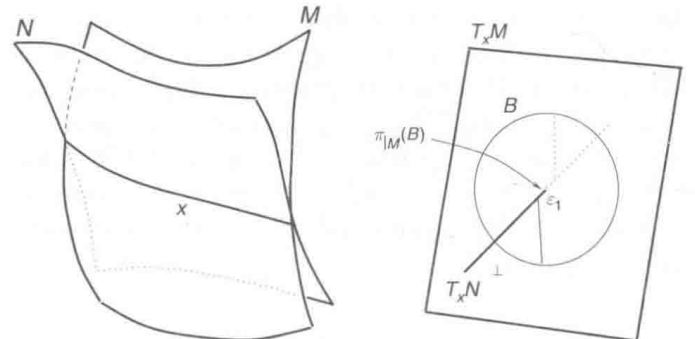


Figure 2 Almost-nontransversality of M and N .

The “bad” set $\Delta(f, B_r, \Lambda)$ is called the set of Λ -almost critical values of f (restricted to B_r). Our purpose is to show that one can control its size in terms of k and Λ . However, before explicitly stating quantitative results, let us precise what we understand by “big set” or by “size of a set.”

Measure and Dimensions

We have a very natural way to measure a subset A of a metric space. To do this, we consider $\alpha \geq 0$ a real number and we denote

$$\mathcal{A}_\nu = \left\{ (D_i)_{i \in \mathbb{N}}; A \subset \bigcup_{i \in \mathbb{N}} D_i \text{ and } |D_i| \leq \nu \right\}$$

where $|D_i|$ is the diameter of D_i ,

$$\mathcal{H}_\nu^\alpha(A) = \inf \left\{ \sum_{i \in \mathbb{N}} |D_i|^\alpha; (D_i)_{i \in \mathbb{N}} \in \mathcal{A}_\nu \right\}$$

and

$$\mathcal{H}^\alpha(A) = \lim_{\nu \rightarrow 0} \mathcal{H}_\nu^\alpha(A) \in \mathbb{R} \cup \{\infty\}$$

$\mathcal{H}^\alpha(A)$ is called the α -dimensional Hausdorff measure of A . It appears that when $\mathcal{H}^\alpha(A) \neq \infty$, $\mathcal{H}^{\alpha'}(A) = 0$ for $\alpha' > \alpha$, and when $\mathcal{H}^\alpha(A) \neq 0$, $\mathcal{H}^{\alpha'}(A) = \infty$ for $\alpha' < \alpha$. This gives rise to the following definition of the Hausdorff dimension of A :

$$\dim_{\mathcal{H}}(A) = \inf \{ \alpha; \mathcal{H}^\alpha(A) = 0 \} \\ = \sup \{ \alpha; \mathcal{H}^\alpha(A) = \infty \}$$

The Hausdorff dimension generalizes the classical notions of dimension, for instance, when A is a subset of \mathbb{R}^n , $\dim_{\mathcal{H}}(A) \leq n$, a d -dimensional manifold has Hausdorff dimension d , and $\mathcal{H}^n(A)$ is the same as the Lebesgue measure \mathcal{L}_n of A (for a very large class of subset A , which we do not describe here. For more details on geometric measure theory, see Falconer (1986) and Federer (1969)).

Another convenient notion of dimension is the (metric) entropy dimension. Let us briefly define it. For a bounded subset A in some metric space and a real number $\alpha > 0$, we denote $M(\alpha, A)$ the minimal number of closed balls of radius $\leq \alpha$, covering A . $H_\alpha(A) = \log_2(M(\alpha, A))$ is called the α -entropy of the set A . This terminology was introduced in Kolmogorov and Tihomirov (1961) and reflects the fact that $H_\alpha(A)$ is the amount of information needed to digitally memorize A with accuracy α . The

entropy dimension of A , $\dim_e(A)$, is the order of $M(\alpha, A)$ as $\alpha \rightarrow 0$. Precisely,

$$\dim_e(A) = \limsup_{\alpha \rightarrow 0} \frac{\log(M(\alpha, A))}{\log(1/\alpha)} \\ = \inf \{ \delta; M(\alpha, A) \leq (1/\alpha)^\delta, \\ \text{for sufficiently small } \alpha \}$$

We clearly have

$$\dim_{\mathcal{H}}(A) \leq \dim_e(A)$$

For any bounded set A in \mathbb{R}^n , we can bound $M(\alpha, A)$ from above by a polynomial in $1/\alpha$ (see Ivanov (1975) and Yomdin and Comte (2004)):

$$M(\alpha, A) \leq c(n) \sum_{i=0}^n V_i(A) (1/\alpha)^i$$

where $c(n)$ only depends on n and $V_i(A)$ (the i th variation of the set A) is the mean value, with respect to P (for a suitable measure), of the number of connected components of $A \cap P$, with P an affine $(n-i)$ -dimensional space of \mathbb{R}^n .

Since for A contained in a d -dimensional manifold, $V_i(A) = 0$ for $i > d$, we deduce from this inequality that in this case $M(\alpha, A)$ is bounded from above by a polynomial of degree $\leq d$ in $1/\alpha$.

Our goal is to explain that we can be more precise than this general inequality when A is a set of critical or almost-critical values of a C^k mapping.

Transversality Is a Generic Situation

The results in this section concern critical values, and not almost-critical values. They show that a “generic” point of the target space is not a critical value, and the more regular, the mapping the smaller the set of critical values. Such theorems relating the regularity of a mapping and the size of its critical values are called Morse–Sard type theorems (see Sard (1942, 1958, 1965)). The simplest theorem in this direction is the following:

Theorem 1 (C^∞ Morse–Sard theorem) (Morse 1939, Sard 1942, Holm 1987). *Let $f: \mathbb{R}^n \rightarrow \mathbb{R}^p$ be a C^∞ -regular mapping. Then $\mathcal{H}^p(\Delta(f, B_r)) = 0$, where $\Delta(f, B_r) = f(\Sigma(f, B_r))$ and $\Sigma(f, B_r)$ is the set of points $x \in B_r$ where $\text{rank}(Df_x) < p$.*

The set $\Delta(f, B_r)$ is the image, under f , of the points of the ball B_r in the source space at which f is not submersive, that is, the set of critical values of f . Consequently, the Morse–Sard theorem ensures that for almost all points y in the target space, $f^{-1}(\{y\})$ is either empty or a smooth submanifold of the source space of dimension $n - p$.

Note that $\Delta(f, B_r) = \Delta(f, B_r, \Lambda)$ for some convenient $\Lambda = (\epsilon_1, \dots, \epsilon_p)$ with $\epsilon_p = 0$, because $x \mapsto l_i(Df_{(x)})$ is bounded on B_r , for all $i \in \{1, \dots, p\}$.

Now, we can concentrate our attention on more singular points than the critical ones, those at which the rank ρ of f is prescribed. Let us denote such points by $\Delta^\rho(f, B_r)$, for $\rho < p$. By definition, $\Delta^\rho(f, B_r) = f(\Sigma^\rho(f, B_r))$, where $\Sigma^\rho(f, B_r) = \{x \in B_r \subset \mathbb{R}^n; \text{rank}(Df_{(x)}) \leq \rho\}$. With these notations, the result for rank- r critical values is the following:

Theorem 2 (C^k Morse–Sard theorem for rank- r critical values) (Federer 1969). *Let $f: \mathbb{R}^n \rightarrow \mathbb{R}^p$ be a C^k -regular mapping. Then $\mathcal{H}^{\rho+(n-\rho)/k}(\Delta^\rho(f, B_r)) = 0$. In particular,*

$$\dim_{\mathcal{H}}(\Delta^\rho(f, B_r)) \leq \rho + \frac{n-\rho}{k}$$

One can produce examples showing that the bound of Theorem 2 is the sharpest one (see Comte (1996), Whitney (1935), Grinberg (1985), and Yomdin and Comte (2004)).

We note that Theorem 1 is a corollary of Theorem 2 (just replace k by ∞ and ρ by $p-1$ in Theorem 2). This result tells nothing about the entropy dimension of $\Delta^\rho(f, B_r)$; in the next section, we will bound the growth of entropy of almost-critical values.

Almost-Transversality Is Almost Generic

In this section, $f: \mathbb{R}^n \rightarrow \mathbb{R}^p$ is a C^k mapping. We denote by K a Lipschitz constant of $D^{k-1}f$ on B_r and by $R_k(f)$ the quantity $(K/(k-1)!) \cdot r^k$. We have:

Theorem 3 (C^k quantitative Morse–Sard theorem) (Yomdin 1983 Yomdin and Comte 2004). *Let $f: \mathbb{R}^n \rightarrow \mathbb{R}^p$ be a C^k mapping, $\Lambda = (\epsilon_1, \dots, \epsilon_p)$, $\epsilon_1 \geq \dots \geq \epsilon_p$, and let us denote $\epsilon_0 = 1$. We have (for $\alpha \leq R_k(f)$):*

$$\begin{aligned} M(\alpha, \Delta(f, B_r, \Lambda)) \\ \leq C \cdot \sum_{i=0}^p \epsilon_0 \cdots \epsilon_i \left(\frac{r}{\alpha}\right)^i \left(\frac{R_k(f)}{\alpha}\right)^{(n-i)/k} \end{aligned}$$

where C is a constant depending only on n, p , and k .

As a corollary, one can bound the entropy dimension of $\Delta^\rho(f, B_r)$ by $\rho + (n-\rho)/k$, and hence its Hausdorff dimension, again finding Theorem 2: we just have to put $\epsilon_{\rho+1} = 0$ and $\epsilon_1, \dots, \epsilon_\rho$ large enough, that is, $\epsilon_i \geq \lambda_i(Df_{(x)})$, for all $x \in B_r$, in Theorem 3, to obtain:

Theorem 4 (C^k entropy Morse–Sard theorem) (Yomdin 1983 Yomdin and Comte 2004). *Let $f: \mathbb{R}^n \rightarrow \mathbb{R}^p$ be a C^k mapping, let us denote $\epsilon_0 = 1$*

and $\epsilon_i = \sup \{\lambda_i(Df_{(x)}); x \in B_r\}$, for $i \in \{1, \dots, p\}$. We have (for $\alpha \leq R_k(f)$):

$$M(\alpha, \Delta^\rho(f, B_r)) \leq C \cdot \sum_{i=0}^p \epsilon_0 \cdots \epsilon_i \left(\frac{r}{\alpha}\right)^i \left(\frac{R_k(f)}{\alpha}\right)^{(n-i)/k}$$

where C is a constant depending only on n, p , and k . In particular,

$$\dim_{\mathcal{H}}(\Delta^\rho(f, B_r)) \leq \dim_e(\Delta^\rho(f, B_r)) \leq \rho + \frac{n-\rho}{k}$$

Again we have examples showing that this bound is sharp (see Yomdin and Comte 2004).

Furthermore, the mapping f in Theorems 2–4 may be of real differentiability class (Hölder smoothness class C^k), with the same conclusions in these theorems. That is, k may be a real number written as $k = p + \beta$ with $\beta \in [0, 1]$, $p \in \mathbb{N} \setminus \{0\}$, and f is C^k means that f is p times differentiable and there exists a constant $C > 0$ such that for all $x, y \in B_r$, $\|D^p f_{(x)} - D^p f_{(y)}\| \leq C \cdot \|x - y\|^\beta$ (see Yomdin and Comte (2004)).

Examples

Let us denote by A the set of real polynomial mappings of degree d and of the following type:

$$x \mapsto Q(a, x) = 1 + \sum_{j=1}^d a_j x^j$$

with $a = (a_1, \dots, a_d)$ and $\|a\| \leq 1$ (where $\|\cdot\|$ is the Euclidean norm of \mathbb{R}^d). We identify the set A with $B^d(0, 1) = \{a \in \mathbb{R}^d; \|a\| \leq 1\}$.

We want to bound the α -entropy of the set of such polynomials for which the real roots are multiple or almost multiple.

We denote by V the set $V = \{(a, x) \in \mathbb{R}^{d+1}; Q(a, x) = 0\}$. At points (a, x) of V with $\nabla Q_{(a, x)} \neq 0$, V is a C^∞ manifold of codimension 1 of \mathbb{R}^{d+1} . We denote by $V^{\text{reg}} = \{(a, x) \in V; \nabla Q_{(a, x)} \neq 0\}$ and by $V^{\text{sing}} = \{(a, x) \in V; \nabla Q_{(a, x)} = 0\} = V \setminus V^{\text{reg}}$. By Whitney (1957), V^{sing} is a union of smooth manifolds of dimension $\leq d-1$.

A root x of a polynomial $Q(a, \cdot)$ is multiple if and only if

$$Q(a, x) = \frac{\partial Q}{\partial x}(a, x) = 0$$

Consequently, the set A^Σ of polynomials of A with multiple roots is $\pi(V^{\text{sing}}) \cup \Delta(\pi|_{V^{\text{reg}}})$, where $\pi: \mathbb{R}^{d+1} \rightarrow \mathbb{R}^d$ is the standard projection $\pi(a, x) = a$, and $\Delta(\pi|_{V^{\text{reg}}})$ is the set $\{(a, x) \in V^{\text{reg}}; 0x \subset T_{(a, x)} V^{\text{reg}}\}$ of critical values of $\pi|_{V^{\text{reg}}}$. By Sard's theorem

(Theorem 2), $\dim_{\mathcal{H}}(\Delta(\pi|_{V^{\text{reg}}})) \leq d-1$. Since $\dim_{\mathcal{H}}(\pi(V^{\text{sing}})) \leq d-1$, we obtain: $\dim_{\mathcal{H}}(A^{\Sigma}) \leq d-1$: thus, having distinct roots is a generic property.

Let, as above, $\Lambda = (\epsilon_1, \dots, \epsilon_d)$ with $\epsilon_1 \geq \dots \geq \epsilon_d$ and $\epsilon_0 = 1$. A root x of a polynomial $Q(a, \cdot) \in A$ is said to be Λ -almost multiple if and only if $Q(a, x) = 0$ and $V \not\perp_x^{\Lambda} O_x$, that is, $(a, x) \in V^{\text{sing}}$ or $\sin(T_{(a,x)} V^{\text{reg}}, O_x) \leq \epsilon_d$. This condition only concerns ϵ_d and we can take $\epsilon_1 = \dots = \epsilon_{d-1} = 1$. We denote $A^{\Sigma, \Lambda}$ to be the set of polynomials of A with (at least) a Λ -almost multiple root. By Theorem 3,

$$M(\alpha, A^{\Sigma, \Lambda} \setminus \pi(V^{\text{sing}})) \leq C \cdot \left[\sum_{i=0}^{d-1} \left(\frac{1}{\alpha} \right)^i + \epsilon_d \cdot \left(\frac{1}{\alpha} \right)^d \right]$$

But $\pi(V^{\text{sing}})$ being a finite union of manifolds of dimension at most $d-1$, we finally obtain

$$M(\alpha, A^{\Sigma, \Lambda}) \leq C' \cdot \left[\sum_{i=0}^{d-1} \left(\frac{1}{\alpha} \right)^i + \epsilon_d \cdot \left(\frac{1}{\alpha} \right)^d \right]$$

Thus, having no Λ -almost multiple root is Λ -almost a generic property. In Figure 3, we represent V for $d=3$ and $a_3=1$,

$$W = \left\{ (a, x) \in \mathbb{R}^{d+1}; \frac{\partial Q}{\partial x}(a, x) = 0 \right\}$$

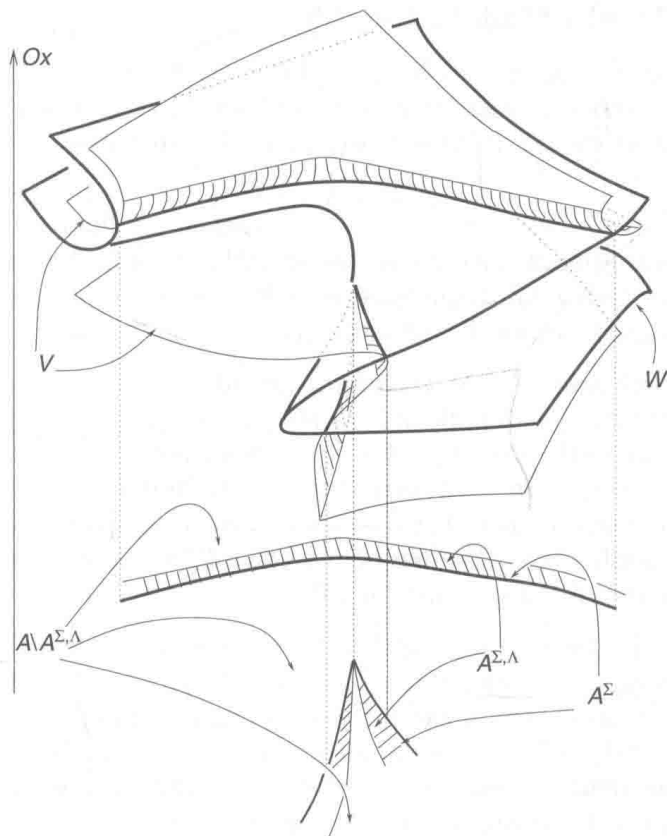


Figure 3 The space of polynomials of type $1 + a_1x + a_2x^2 + x^3$ with almost-multiple roots.

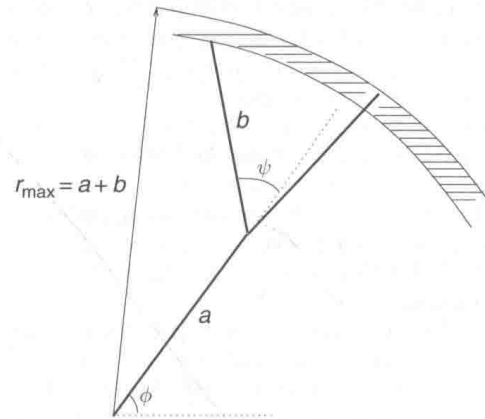


Figure 4 Almost-critical points of the distance function of P to the origin.

The next example comes from robotics: let us consider a planar robotic manipulator consisting of two jointed bars of length a and b , as presented in Figure 4. We may parametrize the positions of the endpoint P of this device by the angles ϕ and ψ (see Figure 4). Now the distance r from the origin to P is $r^2 = \|P\|^2 = a^2 + b^2 + 2ab \cos(\psi)$. The critical points of r are given by

$$\frac{dr}{d\psi}(\psi) = -2ab \sin(\psi) = 0$$

and correspond to the circle $\psi = 0$. The critical value of r is $a + b$. Near these critical positions, the control of r with respect to ψ is poor; we would like to avoid those near-critical values. Given $\epsilon > 0$, the condition

$$\left| \frac{dr}{d\psi}(\psi) \right| \leq \epsilon$$

implies $|\psi| \leq \arcsin(\epsilon/2ab)$, and the ϵ -near-critical values of r are

$$r_{\max}^2 - r^2 \leq 2ab[1 - \cos(\arcsin(\epsilon/2ab))]$$

where r_{\max} is $a + b$; thus, they are contained in an interval of length $\leq c \cdot \epsilon^2 / (4ab \cdot r_{\max})$, and $M(\alpha, \Delta(r, \epsilon)) \leq c \cdot \epsilon^2 / (4ab \cdot r_{\max} \cdot \alpha)$ (Theorem 3 gives $M(\alpha, \Delta(r, \epsilon)) \leq C(1 + \epsilon/\alpha)$).

See also: Entanglement; Entanglement Measures; Quantum Entropy; Singularity and Bifurcation Theory.

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Equivariant Cohomology and the Cartan Model

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Introduction

If a compact Lie group G acts on a manifold M , the space M/G of orbits of the action is usually a singular space. Nonetheless, it is often possible to develop a “differential geometry” of the orbit space in terms of appropriately defined equivariant objects on M . This article is mostly concerned with “differential forms on M/G .” A first idea would be to work with the complex of “basic” forms on M , but for many purposes this complex turns out to be too small. A much more useful complex of equivariant differential forms on M was introduced by Cartan (1950). In retrospect, Cartan's approach presented a differential form model for the equivariant cohomology of M , as defined by A Borel (1960). Borel's construction replaces the quotient M/G by a better-behaved (but usually infinite-dimensional) homotopy quotient M_G , and Cartan's complex should be viewed as a model for forms on M_G .

One of the features of equivariant cohomology are the localization formulas for the integrals of equivariant cocycles. The first instance of such an integration formula was the “exact stationary phase formula,” discovered by Duistermaat and Heckman. This formula was quickly recognized by Berline and Vergne (1983) and Atiyah and Bott (1984), as a localization principle in equivariant cohomology. Today, equivariant localization is a basic tool in mathematical physics, with numerous applications.

This article begins with Borel's topological definition of equivariant cohomology, then proceeds to describe H Cartan's more algebraic approach, and concludes with a discussion of localization principles.

As additional references for the material covered here, we particularly recommend books by Berline, Getzler, and Vergne (1992) and Guillemin and Sternberg (1999).

Borel's Model of $H_G(M)$

Let G be a topological group. A G -space is a topological space M on which G acts by transformations $g \mapsto a_g$, in such a way that the action map

$$a : G \times M \rightarrow M \quad [1]$$

is continuous. An important special case of G -spaces are principal G -bundles $E \rightarrow B$, that is, G -spaces locally isomorphic to products $U \times G$.

Definition 1 A classifying bundle for G is a principal G -bundle $EG \rightarrow BG$, with the following universal property: for any principal G -bundle $E \rightarrow B$, there is a map $f : B \rightarrow BG$, unique up to homotopy, such that E is isomorphic to the pullback bundle f^*EG . The map f is known as a “classifying map” of the principal bundle.

To be precise, the base spaces of the principal bundles considered here must satisfy some technical condition. For a careful discussion, see Husemoller (1994). Classifying bundles exist for all G (by a construction due to Milnor (1956)), and are unique up to G -homotopy equivalence.

It is a basic fact that principal G -bundles with contractible total space are classifying bundles.

Examples 2

- (i) The bundle $R \rightarrow R/\mathbb{Z} = S^1$ is a classifying bundle for $G = \mathbb{Z}$.
- (ii) Let \mathcal{H} be a separable complex Hilbert space, $\dim \mathcal{H} = \infty$. It is known that unit sphere $S(\mathcal{H})$ is contractible. It is thus a classifying $U(1)$ -bundle, with the projective space $P(\mathcal{H})$ as base. More generally, the Stiefel manifold $St(k, \mathcal{H})$ of unitary k -frames is a classifying $U(k)$ -bundle, with base the Grassmann manifold $Gr(k, \mathcal{H})$ of k -planes.
- (iii) Any compact Lie group G arises as a closed subgroup of $U(k)$, for k sufficiently large. Hence, the Stiefel manifold $St(k, \mathcal{H})$ also serves as a model for EG .
- (iv) The based loop group $G = L_0K$ of a connected Lie group K acts by gauge transformations on the space of connections $\mathcal{A}(S^1) = \Omega^1(S^1, \mathfrak{k})$. This is a classifying bundle for L_0K , with base K . The quotient map takes a connection to its holonomy.

For any commutative ring R (e.g., $\mathbb{Z}, \mathbb{R}, \mathbb{Z}_2$), let $H(\cdot; R)$ denote the (singular) cohomology with coefficients in R . Recall that $H(\cdot; R)$ is a graded commutative ring under cup product.

Definition 3 The equivariant cohomology $H_G(M) = H_G(M; R)$ of a G -space M is the cohomology ring of its homotopy quotient $M_G = EG \times_G M$:

$$H_G(M; R) = H(M_G; R) \quad [2]$$

Equivariant cohomology is a contravariant functor from the category of G -spaces to the category of R -modules. The G -map $M \rightarrow \text{pt}$ induces an algebra homomorphism from $H_G(\text{pt}) = H(BG)$ to $H_G(M)$. In this way, $H_G(M)$ is a module over the ring $H(BG)$.

Example 4 (Principal G -bundles). Suppose $E \rightarrow B$ is a principal G -bundle. The homotopy quotient E_G may be viewed as a bundle $E \times_G EG$ over B . Since the fiber is contractible, there is a homotopy equivalence

$$E_G \simeq B \quad [3]$$

and therefore $H_G(E) = H(B)$.

Example 5 (Homogeneous spaces). If K is a closed subgroup of a Lie group G , the space EG may be viewed as a model for EK , with $BK = EG/K = EG \times_K (G/K)$. Hence,

$$H_G(G/K) = H(BK) \quad [4]$$

Let us briefly describe two of the main techniques for computing $H_G(M)$.

1. *Leray spectral sequences.* If R is a field, the equivariant cohomology may be computed as the E_∞ term of the spectral sequence for the fibration $M_G \rightarrow BG$. If BG is simply connected (as is the

case for all compact connected Lie groups), the E_2 -term of the spectral sequence reads

$$E_2^{p,q} = H^p(BG) \otimes H^q(M) \quad [5]$$

2. *Mayer–Vietoris sequences.* If $M = U_1 \cup U_2$ is a union of two G -invariant open subsets, there is a long exact sequence

$$\begin{aligned} \cdots \rightarrow H_G^k(M) \rightarrow H_G^k(U_1) \oplus H_G^k(U_2) \rightarrow \\ \rightarrow H_G^k(U_1 \cap U_2) \rightarrow H_G^{k+1}(M) \rightarrow \cdots \end{aligned}$$

More generally, associated to any G -invariant open cover, there is a spectral sequence converging to $H_G(M)$.

Example 6 Consider the standard $U(1)$ -action on S^2 by rotations. Cover S^2 by two open sets U_\pm , given as the complement of the south pole and north pole, respectively. Since $U_+ \cap U_-$ retracts onto the equatorial circle, on which $U(1)$ acts freely, its equivariant cohomology vanishes except in degree 0. On the other hand, U_\pm retract onto the poles p_\pm . Hence, by the Mayer–Vietoris sequence the map $H_{U(1)}^k(S^2) \cong H_{U(1)}^k(p_+) \oplus H_{U(1)}^k(p_-)$ given by pullback to the fixed points is an isomorphism for $k > 0$. Since the pullback map is a ring homomorphism, we conclude that $H_{U(1)}(S^2; R)$ is the commutative ring generated by two elements x_\pm of degree 2, subject to a single relation $x_+x_- = 0$.

\mathfrak{g} -Differential Algebras

Let G be a Lie group, with Lie algebra \mathfrak{g} . A G -manifold is a manifold M together with a G -action such that the action map [1] is smooth. We would like to introduce the concept of equivariant differential forms on M . This complex should play the role of differential forms on the infinite-dimensional space M_G . In Cartan's approach, the starting point is an algebraic model for the differential forms on the classifying bundle EG .

The algebraic machinery will only depend on the infinitesimal action of G . It is therefore convenient to introduce the following concept.

Definition 7 Let \mathfrak{g} be a finite-dimensional Lie algebra. A \mathfrak{g} -manifold is a manifold M , together with a Lie algebra homomorphism $a: \mathfrak{g} \rightarrow \mathfrak{X}(M)$, $\xi \mapsto a_\xi$ into the Lie algebra of vector fields on M , such that the map $\mathfrak{g} \times M \rightarrow TM$, $(\xi, m) \mapsto a_\xi(m)$ is smooth.

Any G -manifold M becomes a \mathfrak{g} -manifold by taking a_ξ to be the generating vector field

$$a_\xi(m) := \left. \frac{d}{dt} \right|_{t=0} a_{\exp(-t\xi)}(m) \quad [6]$$

Conversely, if G is simply connected, and M is a \mathfrak{g} -manifold for which all of the vector fields a_ξ are complete, the \mathfrak{g} -action integrates uniquely to an action of the group G .

The de Rham algebra $(\Omega(M), d)$ of differential forms on a \mathfrak{g} -manifold M carries graded derivations $L_\xi = L(a_\xi)$ (Lie derivatives, degree 0) and $\iota_\xi = \iota(a_\xi)$ (contractions, degree -1). One has the following graded commutation relations:

$$[d, d] = 0, \quad [L_\xi, d] = 0, \quad [\iota_\xi, d] = L_\xi \quad [7]$$

$$[\iota_\xi, \iota_\eta] = 0, \quad [L_\xi, L_\eta] = L_{[\xi, \eta]_\mathfrak{g}}, \quad [L_\xi, \iota_\eta] = \iota_{[\xi, \eta]_\mathfrak{g}} \quad [8]$$

More generally, the following definitions are introduced.

Definition 8 A \mathfrak{g} -differential algebra (\mathfrak{g} -da) is a commutative graded algebra $A = \bigoplus_{n=0}^\infty A^n$, equipped with graded derivations d, L_ξ, ι_ξ of degrees 1, 0, -1 (where L_ξ, ι_ξ depend linearly on $\xi \in \mathfrak{g}$), satisfying the graded commutation relations [7] and [8].

Definition 9 For any \mathfrak{g} -da A , one defines the horizontal subalgebra $\mathcal{A}_{\text{hor}} = \bigcap_\xi \ker(\iota_\xi)$, the invariant subalgebra $\mathcal{A}^\mathfrak{g} = \bigcap_\xi \ker(L_\xi)$, and the basic subalgebra $\mathcal{A}_{\text{basic}} = \mathcal{A}_{\text{hor}} \cap \mathcal{A}^\mathfrak{g}$.

Note that the basic subalgebra is a differential subcomplex of A .

Definition 10 A connection on a \mathfrak{g} -da is an invariant element $\theta \in A^1 \otimes \mathfrak{g}$, with the property $\iota_\xi \theta = \xi$. The curvature of a connection is the element $F^\theta \in A^2 \otimes \mathfrak{g}$ given as $F^\theta = d\theta + (1/2)[\theta, \theta]_\mathfrak{g}$.

\mathfrak{g} -da's \mathcal{A} admitting connections are the algebraic counterparts of (smooth) principal bundles, with $\mathcal{A}_{\text{basic}}$ playing the role of the base of the principal bundle.

Weil Algebra

The Weil algebra $W\mathfrak{g}$ is the algebraic analog to the classifying bundle EG . Similar to EG , it may be characterized by a universal property:

Theorem 11 *There exists a \mathfrak{g} -da $W\mathfrak{g}$ with connection θ_W , having the following universal property: if \mathcal{A} is a \mathfrak{g} -da with connection θ , there is a unique algebra homomorphism $c: W\mathfrak{g} \rightarrow \mathcal{A}$ taking θ_W to θ .*

Clearly, the universal property characterizes $W\mathfrak{g}$ up to a unique isomorphism. To get an explicit construction, choose a basis $\{e_a\}$ of \mathfrak{g} , with dual basis $\{e^a\}$ of \mathfrak{g}^* . Let $y^a \in \wedge^1 \mathfrak{g}^*$ be the corresponding

generators of the exterior algebra, and $v^a \in S^1 \mathfrak{g}^*$ the generators of the symmetric algebra. Let

$$W^n \mathfrak{g} = \bigoplus_{2i+j=n} S^i \mathfrak{g}^* \otimes \wedge^j \mathfrak{g}^* \quad [9]$$

carry the differential

$$dy^a = v^a + \frac{1}{2} f_{bc}^a y^b y^c \quad [10]$$

$$dv^a = -f_{bc}^a v^b y^c \quad [11]$$

where $f_{bc}^a = \langle e^a, [e_b, e_c]_\mathfrak{g} \rangle$ are the structure constants of \mathfrak{g} . Define the contractions $\iota_a = \iota_{e_a}$ by

$$\iota_a y^b = \delta_a^b, \quad \iota_a v^b = 0 \quad [12]$$

and let $L_a = [d, \iota_a]$. Then L_a are the generators for the adjoint action on $W\mathfrak{g}$. The element $\theta_W = y^a \otimes e_a \in W^1 \mathfrak{g} \otimes \mathfrak{g}$ is a connection on $W\mathfrak{g}$. Notice that we could also use y^a and dy^a as generators of $W\mathfrak{g}$. This identifies $W\mathfrak{g}$ with the Koszul algebra, and implies:

Theorem 12 *$W\mathfrak{g}$ is acyclic, that is, the inclusion $\mathbb{R} \rightarrow W\mathfrak{g}$ is a homotopy equivalence.*

Acyclicity of $W\mathfrak{g}$ corresponds to the contractibility of the total space of EG .

The basic subalgebra of $W\mathfrak{g}$ is equal to $(S\mathfrak{g}^*)^\mathfrak{g}$, and the differential restricts to zero on this subalgebra, since d changes parity. Hence, if \mathcal{A} is a \mathfrak{g} -da with connection, the characteristic homomorphism $c: W\mathfrak{g} \rightarrow \mathcal{A}$ induces an algebra homomorphism, $(S\mathfrak{g}^*)^\mathfrak{g} \rightarrow H(\mathcal{A}_{\text{basic}})$. This homomorphism is independent of θ :

Theorem 13 *Suppose θ_0, θ_1 are two connections on a \mathfrak{g} -da \mathcal{A} . Then their characteristic homomorphisms $c_0, c_1: W\mathfrak{g} \rightarrow \mathcal{A}$ are \mathfrak{g} -homotopic. That is, there is a chain homotopy intertwining contractions and Lie derivatives.*

Remark 14 One obtains other interesting examples of \mathfrak{g} -da's if one drops the commutativity assumption from the definition. For instance, suppose \mathfrak{g} carries an invariant scalar product. Let $\text{Cl}(\mathfrak{g})$ be the corresponding Clifford algebra, and $U(\mathfrak{g})$ the enveloping algebra. The noncommutative Weil algebra (introduced by Alekseev and Meinrenken 2002)

$$W\mathfrak{g} = U\mathfrak{g} \otimes \text{Cl}(\mathfrak{g}) \quad [13]$$

is a (noncommutative) \mathfrak{g} -da, with the derivations d, L_a, ι_a defined on generators by the same formulas as for $W\mathfrak{g}$.

Equivariant Cohomology of \mathfrak{g} -da's

In analogy to $H_G(M) := H(M_G)$, we now declare:

Definition 15 The equivariant cohomology algebra of a \mathfrak{g} -da \mathcal{A} is the cohomology of the differential algebra $\mathcal{A}_{\mathfrak{g}} := (W\mathfrak{g} \otimes \mathcal{A})_{\text{basic}}$:

$$H_{\mathfrak{g}}(\mathcal{A}) := H(\mathcal{A}_{\mathfrak{g}}) \quad [14]$$

The equivariant cohomology $H_{\mathfrak{g}}(\mathcal{A})$ has functorial properties parallel to those of $H_G(M)$. In particular, $H_{\mathfrak{g}}(\mathcal{A})$ is a module over

$$H_{\mathfrak{g}}(\{0\}) = H((W\mathfrak{g})_{\text{basic}}) = (S\mathfrak{g}^*)^{\mathfrak{g}} \quad [15]$$

Theorem 16 Suppose \mathcal{A} is a \mathfrak{g} -da with connection θ , and let $c: W\mathfrak{g} \rightarrow \mathcal{A}$ be the characteristic homomorphism. Then

$$W\mathfrak{g} \otimes \mathcal{A} \rightarrow \mathcal{A}, \quad w \otimes x \mapsto c(w)x \quad [16]$$

is a \mathfrak{g} -homotopy equivalence, with \mathfrak{g} -homotopy inverse the inclusion

$$\mathcal{A} \rightarrow W\mathfrak{g} \otimes \mathcal{A}, \quad x \mapsto 1 \otimes x \quad [17]$$

In particular, there is a canonical isomorphism

$$H(\mathcal{A}_{\text{basic}}) \cong H_{\mathfrak{g}}(\mathcal{A}) \quad [18]$$

Proof By Theorem 13, the automorphism $w \otimes x \mapsto 1 \otimes c(w)x$ of $W\mathfrak{g} \otimes \mathcal{A}$ is \mathfrak{g} -homotopic to the identity map. \square

The above definition of the complex $\mathcal{A}_{\mathfrak{g}}$ is often referred to as the Weil model of equivariant cohomology, while the term Cartan model is reserved for a slightly different description of $\mathcal{A}_{\mathfrak{g}}$. Identify the space $(S\mathfrak{g}^* \otimes \mathcal{A})^{\mathfrak{g}}$ with the algebra of equivariant \mathcal{A} -valued polynomial functions $\alpha: \mathfrak{g} \rightarrow \mathcal{A}$. Define a differential $d_{\mathfrak{g}}$ on this space by setting

$$(d_{\mathfrak{g}}\alpha)(\xi) = d(\alpha(\xi)) - \iota_{\xi}\alpha(\xi) \quad [19]$$

Theorem 17 (H Cartan). The natural projection $W\mathfrak{g} \otimes \mathcal{A} \rightarrow S\mathfrak{g}^* \otimes \mathcal{A}$ restricts to an isomorphism of differential algebras, $\mathcal{A}_{\mathfrak{g}} \cong (S\mathfrak{g}^* \otimes \mathcal{A})^{\mathfrak{g}}$.

Suppose \mathcal{A} carries a connection θ . The \mathfrak{g} -homotopy equivalence [16] induces a homotopy equivalence $\mathcal{A}_{\mathfrak{g}} \rightarrow \mathcal{A}_{\text{basic}}$ of the basic subcomplexes. By explicit calculation, the corresponding map for the Cartan model is given by

$$(S\mathfrak{g}^* \otimes \mathcal{A})^{\mathfrak{g}} \rightarrow \mathcal{A}_{\text{basic}}, \quad \alpha \mapsto P_{\text{hor}}^{\theta}(\alpha(F^{\theta})) \quad [20]$$

Here $\alpha(F^{\theta}) \in \mathcal{A}^{\mathfrak{g}}$ is the result of substituting the curvature of θ , and $P_{\text{hor}}: \mathcal{A} \rightarrow \mathcal{A}_{\text{hor}}$ is horizontal projection. On elements of $(S\mathfrak{g}^*)^{\mathfrak{g}} \subset (S\mathfrak{g}^* \otimes \mathcal{A})^{\mathfrak{g}}$,

the map [20] specializes to the Chern–Weil homomorphism.

There is an algebraic counterpart of the Leray spectral sequence: introduce a filtration

$$F^p \mathcal{A}_{\mathfrak{g}}^{p+q} := \bigoplus_{2i \geq p} (S^i \mathfrak{g}^* \otimes \mathcal{A}^q)^{\mathfrak{g}} \quad [21]$$

Since second term in the equivariant differential [19] raises the filtration degree by 2, it follows that

$$E_2^{p,q} = (S^{p/2} \mathfrak{g}^*)^{\mathfrak{g}} \otimes H^q(\mathcal{A}) \quad [22]$$

for p even, $E_2^{p,q} = 0$ for p odd. In fortunate cases, the spectral sequence collapses at the E_2 -stage (see below).

Equivariant de Rham Theory

We will now restrict ourselves to the case that $\mathcal{A} = \Omega(M)$ is the algebra of differential forms on a G -manifold, where G is compact and connected.

Theorem 18 (Equivariant de Rham theorem). Suppose G is a compact, connected Lie group, and that M is a G -manifold. Then there is a canonical isomorphism

$$H_G(M; \mathbb{R}) \cong H_{\mathfrak{g}}(\Omega(M)) \quad [23]$$

where the left-hand side is the equivariant cohomology as defined by the Borel construction.

Motivated by this result, the notation can be changed slightly; write

$$\Omega_G(M) = (S\mathfrak{g}^* \otimes \Omega(M))^G \quad [24]$$

for the Cartan complex of equivariant differential forms, and d_G for the equivariant differential [19].

Remark 19 Theorem 18 fails, in general, for noncompact Lie groups G . A differential form model for the noncompact case was developed by Getzler (1990).

Example 20 Let (M, ω) be a symplectic manifold, and $a: G \rightarrow \text{Diff}(M)$ a Hamiltonian group action. That is, a preserves the symplectic form, $a_g^* \omega = \omega$, and there exists an equivariant moment map $\Phi: M \rightarrow \mathfrak{g}^*$ such that $\iota_{\xi} \omega + d\langle \Phi, \xi \rangle = 0$. Then the equivariant symplectic form $\omega_G(\xi) := \omega + \langle \Phi, \xi \rangle$ is equivariantly closed.

Example 21 Let G be a Lie group, and denote, respectively, by

$$\theta^L = g^{-1} dg \text{ and } \theta^R = dg g^{-1} \quad [25]$$

the left- and right-invariant Maurer–Cartan forms. Suppose $\mathfrak{g} = \text{Lie}(G)$ carries an invariant scalar product “ \cdot ”, and consider the closed 3-form

$$\phi = \frac{1}{12} \theta^L \cdot [\theta^L, \theta^L] \quad [26]$$

Then

$$\phi_G(\xi) = \phi + \frac{1}{2}(\theta^L + \theta^R) \cdot \xi \quad [27]$$

is a closed equivariant extension for the conjugation action of G . More generally, transgression gives explicit differential forms ϕ_i generating the cohomology ring $H(G) = (\wedge \mathfrak{g}^*)^G$. Closed equivariant extensions of these forms were obtained by Jeffrey (1995), using a construction of Bott–Shulman.

A G -manifold is called equivariantly formal if

$$H_G(M) = (S\mathfrak{g}^*)^G \otimes H(M) \quad [28]$$

as an $(S\mathfrak{g}^*)^G$ -module. Equivalently, this is the condition that the spectral sequence [22] for $H_G(M)$ collapses at the E_2 -term. M is equivariantly formal under any of the following conditions: (1) $H^q(M) = 0$ for q odd, (2) the map $H_G(M) \rightarrow H(M)$ is onto, (3) M admits a G -invariant Morse function with only even indices, and (4) M is a symplectic manifold and the G -action is Hamiltonian. (The last fact is a theorem due to Ginzburg and Kirwan.

Example 22 The conjugation action of a compact Lie group is equivariantly formal, by criterion [2]. In this case, eqn [28] is an isomorphism of algebras.

It is important to note that eqn [28] is not an algebra isomorphism, in general. Already the rotation action of $G = \text{U}(1)$ on $M = S^2$, discussed in Example 6, provides a counter-example.

Theorem 23 (Injectivity). *Suppose T is a compact torus, and M is T -equivariantly formal. Then the pullback map $H_T(M) \rightarrow H_T(M^T)$ to the fixed point set is injective.*

Since the pullback map to the fixed point set is an algebra homomorphism, one can sometimes use this result to determine the algebra structure on $H_T(M)$: let $\alpha_r \in H(M)$ be generators of the ordinary cohomology algebra, and let $(\alpha_r)_T$ be equivariant extensions. Denote by $x_r \in H_T(M^T)$ the pullbacks of $(\alpha_r)_T$ to the fixed point set, and let y_i be a basis of t^* , viewed as elements of $S t^* \subset H_T(M^T)$. Then $H_T(M)$ is isomorphic to the subalgebra of $H_T(M^T)$ generated by the x_r and y_i .

The case of nonabelian compact groups G may be reduced to maximal torus T using the following result. Observe that for any G -manifold M , there is a natural action of the Weyl group $W = N(T)/T$ on $H_T(M)$.

Theorem 24 *The natural restriction map*

$$H_G(M; \mathbb{R}) \rightarrow H_T(M; \mathbb{R})^W \quad [29]$$

onto the Weyl group invariants is an algebra isomorphism.

Remark 25 The Cartan complex [24] may be viewed as a small model for the differential forms on the infinite-dimensional space M_G . In the noncommutative case, there exists an even “smaller” Cartan model, with underlying complex $(S\mathfrak{g}^*)^G \otimes \Omega(M)^G$, involving only invariant differential forms on M (see Alekseev and Meinrenken (2005) and Goresky, Kottwitz, and MacPherson (1998)).

Equivariant Characteristic Forms

Let G be a compact Lie group, and $E \rightarrow B$ a principal G -bundle with connection $\theta \in \Omega^1(E) \otimes \mathfrak{g}$. Suppose the principal G -action commutes with the action of a compact Lie group K on E , and that θ is K -invariant. The K -equivariant curvature of θ is defined as follows:

$$F_K^\theta = d_K \theta + \frac{1}{2}[\theta, \theta] \in \Omega_K^2(E) \otimes \mathfrak{g}$$

By the equivariant version of eqn [20], there is a canonical chain map

$$\Omega_{K \times G}(E) \rightarrow \Omega_K(B) \quad [30]$$

defined by substituting the K -equivariant curvature for the \mathfrak{g} -variable, followed by horizontal projection with respect to θ . The Cartan map [30] is homotopy inverse to the pullback map from $\Omega_K(B)$ to $\Omega_{K \times G}(B)$.

Example 26 The complex $\Omega_{K \times G}(E)$ contains a subcomplex $(S\mathfrak{g}^*)^G$. The restriction of eqn [30] is the equivariant Chern–Weil map

$$(S\mathfrak{g}^*)^G \rightarrow \Omega_K(B) \quad [31]$$

Forms in the image of eqn [31] are equivariantly closed; they are called the K -equivariant characteristic forms of E .

Example 27 Similarly, if $\mathcal{V} \rightarrow B$ is a K -equivariant vector bundle with structure group $G \subset \text{GL}(k)$, one defines the K -equivariant characteristic forms of \mathcal{V} to be those of the corresponding bundle of G -frames in \mathcal{V} .

For instance, suppose \mathcal{V} is an oriented K -equivariant vector bundle of even rank k , with an invariant metric and compatible connection. The Pfaffian defines an invariant polynomial on $\mathfrak{so}(k)$:

$$\zeta \mapsto \det^{1/2}(\zeta/2\pi) \quad [32]$$

(equal to 0 if k is odd). The K -equivariant characteristic form of degree k on B determined by eqn [32] is known as the equivariant Euler form

$$\text{Eul}_K(\mathcal{V}) \in \Omega_K^k(B) \quad [33]$$

Similarly, one defines equivariant Pontrjagin forms of \mathcal{V} , and (for Hermitian vector bundles) equivariant Chern forms.

Example 28 Suppose G is a maximal rank subgroup of the compact Lie group K . The bundle $K \rightarrow K/G$ admits a unique K -invariant connection. Hence, one obtains a canonical chain map $(S\mathfrak{g}^*)^G \rightarrow \Omega_K(K/G)$, realizing the isomorphism $H_K(K/G) \cong (S\mathfrak{g}^*)^G$. In particular, any G -invariant element of \mathfrak{g}^* defines a closed K -equivariant 2-form on K/G . For instance, symplectic forms on coadjoint orbits are obtained in this way.

Suppose M is a G -manifold, and let $Q = E \times_G M$ be the associated bundle. For any K -invariant connection on E , one obtains a chain map

$$\Omega_G(M) \rightarrow \Omega_{K \times G}(E \times M) \rightarrow \Omega_K(Q) \quad [34]$$

by composing the pullback to $E \times M$ with the Cartan map for the principal bundle $E \times M \rightarrow Q$.

Example 29 Suppose (M, ω) is a Hamiltonian G -manifold, with moment map $\Phi: M \rightarrow \mathfrak{g}^*$. The image of $\omega_G = \omega + \Phi$ under the map [34] defines a closed K -equivariant 2-form on Q . This construction is of importance in symplectic geometry, where it arises in the context of Sternberg's minimal coupling.

Equivariant Thom Forms

Let $\pi: \mathcal{V} \rightarrow B$ be a G -equivariant oriented real vector bundle of rank k over a compact base B . There is a canonical chain map, called fiber integration

$$\pi_*: \Omega^\bullet(\mathcal{V})_{\text{cp}} \rightarrow \Omega^{\bullet-k}(B) \quad [35]$$

where the subscript indicates "compact support." It is characterized by the following properties:

- (1) for a form of degree k , the value of its fiber integral at $x \in B$ is equal to the integral over the fiber \mathcal{V}_x , and
- (2)

$$\pi_*(\alpha \wedge \pi^*\beta) = \pi_*\alpha \wedge \beta \quad [36]$$

for all $\alpha \in \Omega(\mathcal{V})_{\text{cp}}$ and $\beta \in \Omega(B)$. Fiber integration extends to G -equivariant differential forms, and commutes with the equivariant differential.

Theorem 30 (Equivariant Thom isomorphism). *Fiber integration defines an isomorphism,*

$$H_G^{\bullet+k}(\mathcal{V})_{\text{cp}} \rightarrow H_G^\bullet(B) \quad [37]$$

An equivariant Thom form for a G -vector bundle is a cocycle $\text{Th}_G(\mathcal{V}) \in \Omega_G^k(\mathcal{V})_{\text{cp}}$, with the property,

$$\pi_*\text{Th}_G(\mathcal{V}) = 1 \quad [38]$$

Given $\text{Th}_G(\mathcal{V})$, the inverse to eqn [37] is realized on the level of differential forms as

$$\Omega_G^\bullet(B) \rightarrow \Omega_G^{\bullet+k}(E), \quad \alpha \mapsto \text{Th}_G(\mathcal{V}) \wedge \pi^*\alpha \quad [39]$$

A beautiful "universal" construction of Thom forms was obtained by Mathai and Quillen (1986). Using eqn [34], it suffices to describe an $\text{SO}(k)$ -equivariant Thom form for the trivial bundle $\mathbb{R}^k \rightarrow \{0\}$. Using multi-index notation for ordered subsets $I \subset \{1, \dots, k\}$,

$$\text{Th}_{\text{SO}(k)}(\mathbb{R}^k)(\zeta) = \frac{e^{-\|x\|^2}}{\pi^{k/2}} \sum_I \epsilon_I \det^{1/2} \left(\frac{\zeta_I}{2} \right) (dx)^{I^c} \quad [40]$$

Here the sum is over all subsets I with $|I|$ even, and I^c is the complement of I . The matrix ζ_I is obtained from ζ by deleting all rows and columns that are not in I , and $\det^{1/2}$ is defined as a Pfaffian. Finally, ϵ_I is the sign of the shuffle permutation defined by I , that is, $(dx)^I(dx)^{I^c} = \epsilon_I dx_1 \cdots dx_k$. As shown by Mathai and Quillen, the form [40] is equivariantly closed, and clearly eqn [38] holds since the top degree part is just a Gaussian. If k is even, the Mathai–Quillen formula can also be written, on the open dense where $\zeta \in \mathfrak{so}(k)$ is invertible, as

$$\text{Th}_{\text{SO}(k)}(\mathbb{R}^k)(\zeta) = \det^{1/2} \left(\frac{\zeta}{2\pi} \right) e^{-\|x\|^2 - \langle dx, \zeta^{-1}(dx) \rangle} \quad [41]$$

The form $\text{Th}_{\text{SO}(k)}(\mathbb{R}^k)$ given by these formulas does not have compact support, but is rapidly decreasing at infinity. One obtains a compactly supported Thom form, by applying an $\text{SO}(k)$ -equivariant diffeomorphism from \mathbb{R}^k onto some open ball of finite radius.

Note that the pullback of eqn [40] to the origin is equal to $\det^{1/2}(\zeta/2\pi)$ (equal to 0 if k is odd). This implies:

Theorem 31 *Let $\iota: B \rightarrow \mathcal{V}$ denote the inclusion of the zero section. Then*

$$\iota^*\text{Th}_G(\mathcal{V}) = \text{Eul}_G(\mathcal{V}) \quad [42]$$

where $\text{Eul}_G(\mathcal{V}) \in \Omega_G^k(B)$ is the equivariant Euler form.

Suppose, M is a G -manifold, and S a closed G -invariant submanifold with oriented normal

bundle ν_S . Choose a G -equivariant tubular neighborhood embedding

$$\nu_S \rightarrow U \subset M \quad [43]$$

and let $\text{PD}_G(S) \in \Omega_G(M)_{cp}$ be the image of $\text{Th}_G(\mathcal{V})$ under this embedding. The form $\text{PD}_G(S)$ has the property

$$\int_M \text{PD}_G(S) \wedge \alpha = \int_S \iota_S^* \alpha \quad [44]$$

for all closed equivariant forms $\alpha \in \Omega_G(M)$. It is called an “equivariant Poincaré dual” of S . By construction, the pullback to S is the equivariant Euler form:

$$\iota_S^* \text{PD}_G(S) = \text{Eul}_G(\nu_S) \quad [45]$$

Equivariant Poincaré duality takes transversal intersections of G -manifolds to wedge products, similar to the nonequivariant case.

Remark 32 In general, the $(Sg^*)^G$ -submodule generated by Poincaré duals of G -invariant submanifolds is strictly smaller than $H_G(M)$. In this sense, the terminology “duality” is misleading.

Localization Theorem

In this section, T will denote a torus. Suppose M is a compact oriented T -manifold. For any component F of the fixed point set of T , the action of T on ν_F fixes only the zero section F . This implies that the normal bundle ν_F has even rank and is orientable. Fix an orientation, and give F the induced orientation.

Since T is compact, the list of stabilizer groups of points in M is finite. Call $\xi \in \mathfrak{t}$ generic if it is not in the Lie algebra of any of these stabilizers, other than T itself. In this case, value $\text{Eul}_T(\nu_F, \xi)$ of the equivariant Euler form is invertible as an element of $\Omega(F)$.

Theorem 33 (Integration formula). *Suppose M is a compact oriented T -manifold, where T is a torus. Let $\alpha \in \Omega_T(M)$ be a closed equivariant form, and let $\xi \in \mathfrak{t}$ be generic. Then*

$$\int_M \alpha(\xi) = \sum_F \int_F \frac{\iota_F^* \alpha(\xi)}{\text{Eul}_T(\nu_F, \xi)} \quad [46]$$

where the sum is over the connected components of the fixed point set.

Rather than fixing ξ , one can also view eqn (46) as an equality of rational functions of $\xi \in \mathfrak{t}$.

Remark 34 The integration formula was obtained by Berline and Vergne (1983), based on ideas of Bott (1967). The topological counterpart, as a “localization principle,” was proved independently by Atiyah

and Bott (1984). More abstract versions of the localization theorem in equivariant cohomology had been proved earlier by Borel, Chiang–Skjelbred and others.

Remark 35 If $\alpha = \text{PD}_T(F) \wedge \beta$, where β is equivariantly closed, the integration formula is immediate from the property [44] of Poincaré duals. The essence of the proof is to reduce to this case.

Remark 36 The localization contributions are particularly nice if $F = \{p\}$ is isolated (which can only happen if $\dim M$ is even). In this case, $\iota_F^* \alpha(\xi)$ is simply the value of the function $\alpha_{[0]}(\xi)$ at p . For the Euler form, one has

$$\text{Eul}(\nu_F, \xi) = (-1)^{\dim M/2} \prod \langle \mu_j(p), \xi \rangle \quad [47]$$

where $\mu_j(p) \in \mathfrak{t}^*$ are the (real) weights of the action on the tangent space $T_p M$. (Here we have chosen an isomorphism $T_p M \cong \mathbb{C}^l$ compatible with the orientation.) Hence, if all fixed points are isolated,

$$\int_M \alpha(\xi) = (-1)^{\dim M/2} \sum_p \frac{\alpha_{[0]}(\xi)(p)}{\prod_j \langle \mu_j(p), \xi \rangle} \quad [48]$$

Example 37 Let M be a compact oriented manifold, and $e(M) = \int_M \text{Eul}(TM)$ its Euler characteristic. Suppose a torus T acts on M . Then

$$e(M) = \sum_F e(F) \quad [49]$$

where the sum is over the fixed point set of T . This follows from the integral of the equivariant Euler form $\alpha(\xi) = \text{Eul}_T(M, \xi)$, by letting $\xi \rightarrow 0$ in the localization formula. In particular, if M admits a circle action with isolated fixed points, the number of fixed points is equal to the Euler characteristic.

In a similar fashion, the localization formula gives interesting expressions for other characteristic numbers of manifolds and vector bundles, in the presence of a circle action. Some of these formulas were discovered prior to the localization formula, see in particular Bott (1967).

Example 38 In this example, we show that for a simply connected, simple Lie group G the 3-form $\phi \in \Omega^3(G)$ defined in eqn [26] is integral, provided “ \cdot ” is taken to be the basic inner product (for which the length squared of the short coroots equals 2). Since any such G is known to contain an $\text{SU}(2)$ subgroup, it suffices to prove this for $G = \text{SU}(2)$. Consider the conjugation action of the maximal torus $T \cong \text{U}(1)$, consisting of diagonal matrices. The fixed point set for this action is T itself. The normal

bundle ν_F is trivial, with T acting on the fiber $\mathfrak{g}/\mathfrak{t}$ by the negative root $-\alpha$. Hence, $\text{Eul}(\nu_F, \xi) = \langle \alpha, \xi \rangle$. Let $\tilde{\alpha} \in \mathfrak{t}$ be the coroot, defined by $\langle \alpha, \tilde{\alpha} \rangle = 2$. By definition, $\langle \alpha, \tilde{\alpha} \rangle = 2$. Let us integrate the T -equivariant extension $\phi_T(\xi)$ (cf. [27]). Its pullback to T is $\theta^T \cdot \xi$, where $\theta^T \in \Omega(T, \mathfrak{t})$ is the Maurer–Cartan form. The integral of θ^T is a generator of the integral lattice, that is, it equals $\tilde{\alpha}$. Thus,

$$\int_{\text{SU}(2)} \phi_T(\xi) = \frac{\int_T \theta^T \cdot \xi}{\langle \alpha, \xi \rangle} = \frac{\tilde{\alpha} \cdot \xi}{\langle \alpha, \xi \rangle} = 1 \quad [50]$$

Duistermaat–Heckman Formulas

In this section, we discuss the Duistermaat–Heckman formula, for the case of isolated fixed points. Let T be a torus, and (M, ω) a compact Hamiltonian T -space, with moment map $\Phi: M \rightarrow \mathfrak{t}^*$. Denote by $\omega_T = \omega + \Phi$ the equivariant extension of ω . Assuming isolated fixed points, the localization formula gives, for all integers $k \geq 0$,

$$\int_M (\omega + \langle \Phi, \xi \rangle)^k = (-1)^n \sum_p \frac{\langle \Phi(p), \xi \rangle^k}{\prod_j \langle \mu_j(p), \xi \rangle} \quad [51]$$

where $n = (1/2) \dim M$. Note that both sides are homogeneous of degree $k - n$ in ξ , but the terms on the right-hand side are only rational functions while the left-hand side is a polynomial. For $k = n$, both sides are independent of ξ , and compute the integral $\int_M \omega^n$. For $k < n$, the integral [51] is zero, and the cancellation of the terms on the right-hand side gives identities among the weights $\mu_j(p)$. Equation [51] also implies

$$\int_M e^{\omega + \langle \Phi, \xi \rangle} = (-1)^n \sum_p \frac{e^{\langle \Phi(p), \xi \rangle}}{\prod_j \langle \mu_j(p), \xi \rangle} \quad [52]$$

Assume, in particular, that $T = \text{U}(1)$, and let $\xi = t\xi_0$, where ξ_0 is the generator of the integral lattice in \mathfrak{t} . Identify $\mathfrak{t} \cong \mathbb{R}$ in such a way that ξ_0 corresponds to $1 \in \mathbb{R}$. Then $H = \langle \Phi, \xi_0 \rangle$ is a Hamiltonian function with periodic flow. Write $a_j(p) = \langle \mu_j(p), \xi_0 \rangle \in \mathbb{Z}$. Then eqn [52] reads

$$\int_M e^{tH} \frac{\omega^n}{n!} = \frac{(-1)^n}{t^n} \sum_p \frac{e^{tH(p)}}{\prod_j a_j(p)} \quad [53]$$

The right-hand side of eqn [53] is the leading term for the stationary phase approximation of the integral on the left. For this reason, eqn [52] is known as the Duistermaat–Heckman exact stationary phase theorem.

Formula [52] has the following consequence for the push-forward of the Liouville measure under the

moment map, the so-called Duistermaat–Heckman measure $H_*(\omega^n/n!)$. Let Θ be the Heaviside measure (i.e., the characteristic measure of the positive real axis).

Theorem 39 (Duistermaat–Heckman). *The push-forward $H_*(\omega^n/n!)$ is piecewise polynomial measure of degree $n - 1$, with singularities at the set of all $H(p)$ for fixed points p of the action. One has the formula*

$$H_*\left(\frac{\omega^n}{n!}\right) = \sum_p \frac{(\lambda - H(p))^{n-1}}{\prod_j a_j(p)} \Theta(\lambda - H(p)) \quad [54]$$

Proof It is enough to show that the Laplace transforms of the two sides are equal. Multiplying by $e^{t\lambda}$ and integrating over λ (take $t < 0$ to ensure convergence of the integral), the resulting identity is just eqn [53]. \square

Remark 40 The theorem generalizes to Hamiltonian actions of higher-rank tori, and also to nonisolated fixed points. See the paper by Guillemin, Lerman, and Sternberg (1988) for a detailed discussion of this formula and of its “quantum analog.”

Equivariant Index Theory

By definition, the Cartan model consists of equivariant forms $\alpha(\xi)$ with polynomial dependence on the equivariant parameter ξ . However, the integration formula holds in much greater generality. For instance, one may consider generalized Cartan complexes (Kumar and Vergne 1993). Here the parameter ξ varies in some invariant open subset of \mathfrak{g} , and the polynomial dependence is replaced by smooth dependence. The use of these more general complexes in equivariant index theory was pioneered by Berline and Vergne (1992).

Assume that M is an even-dimensional, compact oriented Riemannian manifold, equipped with a Spin- c structure. According to the Atiyah–Singer theorem, the index of the corresponding Dirac operator D is given by the formula

$$\text{ind}(D) = \int_M \hat{A}(M) e^{c/2} \quad [55]$$

Here c is the curvature 2-form of the complex line bundle associated to the Spin- c structure, and $\hat{A}(M)$ is the \hat{A} -form. Recall that $\hat{A}(M)$ is obtained by substituting the curvature form in the formal power series expansion of the function $\hat{A}(x) = \det^{1/2}((x/2)/\sinh(x/2))$ on $\mathfrak{so}(n)$.

Suppose now that a compact, connected Lie group G acts on M by isometries, and that the action lifts to the Spin- c bundle. Replacing curvatures with equivariant curvatures, one defines the equivariant form $\hat{A}(M)(\xi)$ and the form $c(\xi)$. Note that $\hat{A}(\xi)$ is only

defined for ξ in a sufficiently small neighborhood of 0, since the function $\hat{A}(x)$ is not analytic for all x .

The G -index of the equivariant Spin- c Dirac operator is a virtual character $g \mapsto \text{ind}(D)(g)$ of the group G . For $g = \exp \xi$ sufficiently small, it is given by the formula

$$\text{ind}(D)(\exp \xi) = \int_M \hat{A}(M)(\xi) e^{c(\xi)/2} \quad [56]$$

For ξ sufficiently small, the fixed point set of g coincides with the set of zeroes of the vector field a_ξ . The localization formula reproduces the Atiyah–Segal formula for $\text{ind}(D)(g)$, as an integral over M^g .

Berline and Vergne (1996) gave similar formulas for the equivariant index of any G -equivariant elliptic operator, and more generally for operators that are transversally elliptic in the sense of Atiyah.

See also: Cohomology Theories; Compact Groups and Their Representations; Hamiltonian Group Actions; K -theory; Lie Groups: General Theory; Mathai–Quillen Formalism; Path-Integrals in Noncommutative Geometry; Stationary Phase Approximation.

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Ergodic Theory

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Introduction

The ergodic theory was developed from the following Poincaré's work, which served as the starting point in the measure theory of dynamical systems in the sense of the study of the properties of motions that take place at “almost all” initial states of a system: let (X, \mathcal{B}, μ) be a probability space and a transformation $T: X \rightarrow X$ preserve μ (i.e., $\mu(T^{-1}A) = \mu(A)$ for any $A \in \mathcal{B}$). If $\mu(A) > 0$, then for almost all points $x \in A$ the orbit $\{T^n x\}_{n \geq 0}$ returns to A infinitely more often (the Poincaré–Caratheodory recurrence theorem).

The main theme of the ergodic theory is to know whether averages of quantities generated in a stationary manner converge. In the classical situation the stationary is described by a measure-preserving transformation T , and one considers averages taken along a sequence f, fT, fT^2, \dots for integrable f . This corresponds to the probabilistic concept of stationarity. Hence, traditionally, the ergodic theory is the qualitative study of iterates of an individual transformation, of one parameter flow of transformations (such as that obtained from the solution of an autonomous ordinary differential equation). We should note that an important purpose behind this theory is to verify significant facts from a statistical point of view (e.g., the law of large numbers, convergence to limit distributions). The oldest branch

of this theory is the study of ergodic theorems. It was started in 1931 by Birkhoff (1931) and von Neumann (1932), having its origins in statistical mechanics. More specifically, the central notion is that of ergodicity, which is intended to capture the idea that a flow is “random” or “chaotic.” In dealing with the motion of molecules, Boltzmann and Gibbs made such hypotheses from the beginning. One of the earliest precise definitions of randomness of a dynamical system was “minimality”: the orbit of almost every point is dense. In order to describe such phenomena in measure-theoretical setting, von Neumann and Birkhoff required the stronger assumption of ergodicity as follows. Let (X, \mathcal{B}, μ) be a measure space and F_t a measurable flow on X . We call F_t ergodic if the only invariant measurable sets are \emptyset or all of X . Here, the invariance of the set A means that $F_t(A) = A$ for all $t \in \mathbb{R}$ and we agree to write $A = B$ if A and B differ by a null set with respect to μ . Note that ergodicity implies minimality if we are on a second countable Borel space. A function $f: X \rightarrow \mathbb{R}$ will be called a “constant of the motion” iff $f \circ F_t = f$ a.e. for each $t \in \mathbb{R}$. Then we see that a flow F_t on X is ergodic iff the only constants of the motion are constant a.e. In case of a measurable transformation T on X , the invariance of the set A means that $T^{-1}A = A$, and the measurable function f is called invariant if $f \circ T = f$ a.e. Then we call T ergodic provided if A is invariant then either $\mu(A) = 0$ or $\mu(A) = 1$; equivalently, any invariant function is constant a.e. (Cornfeld *et al.* 1982). The most basic example where ergodicity can be verified is the following: if M is a compact Riemannian and has negative sectional curvatures at each point, then the geodesic flow on each sphere bundle is ergodic (Hopf–Hadamard). In general, verifying ergodicity can still be very difficult. In the Hamiltonian case, the first step is to pass to an energy surface. For example, Sinai (1970) shows that one has ergodicity on an energy surface of a classical model for molecular motion, that is, a collection of hard spheres in a box.

Ergodic Theorems

Koopman (1931) published the following significant observation: if T is an invertible measure-preserving transformation of a measure space (X, \mathcal{B}, μ) , then the operator U , defined on $L^2(X, \mathcal{B}, \mu)$ by $Uf(x) := f(Tx)$, is unitary. Thus, the association of U with T replaces a nonlinear finite-dimensional problem with a linear infinite-dimensional one. Then von Neumann (1932) showed an intimate connection between measure-preserving transformations and unitary operators (the mean ergodic theorem): let U be a unitary operator on a Hilbert

space \mathcal{H} . Denote by P the orthogonal projection onto the subspace $\mathcal{H}_0 := \{f \in \mathcal{H} | Uf = f\}$. For any $f \in \mathcal{H}$, one has

$$\lim_{N \rightarrow \infty} \left\| \frac{1}{N} \sum_{n=0}^{N-1} U^n f - Pf \right\|_{\mathcal{H}} = 0$$

As a corollary, one can show that if $T: X \rightarrow X$ is an ergodic measure-preserving transformation on a probability space (X, \mathcal{B}, μ) then, for any $f \in L^1(X, \mathcal{B}, \mu)$,

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=0}^{N-1} f(T^n x) = \frac{1}{\mu(X)} \int_X f d\mu$$

in L^1 -norm. We also know that T is ergodic if and only if U has 1 as a simple eigenvalue. In the case of a continuous invertible process, the setting is the following. Let M be a manifold and Ω a volume on M , with μ_Ω the corresponding measure. If F_t is a volume-preserving flow on M , then F_t induces a linear one-parameter group of isometries on $\mathcal{H} = L^2(M, \mu_\Omega)$ by $U_t(f) = f \circ F_{-t}$. Then U_t has 1 as a simple eigenvalue for all t if and only if F_t is ergodic.

On the other hand, Birkhoff (1931) proved the following almost everywhere statement (the pointwise ergodic theorem): for any $f \in L^1(X, \mathcal{B}, \mu)$, there exists a function $\bar{f} \in L^1(X, \mathcal{B}, \mu)$ such that for μ -a.e. x , $\bar{f}T(x) = \bar{f}(x)$ and

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=0}^{N-1} f(T^n x) = \bar{f}(x)$$

In particular, if T is ergodic then μ -a.e. x , $\bar{f}(x) = \int_X f d\mu$. Thus, the Birkhoff theorem allows one to prove the ergodic hypothesis by Boltzmann–Gibbs, that is, the space average of an observable function coincides with its time averages almost everywhere, and guarantees the existence, for almost everywhere, of the mean number of occurrences in any measurable set. On the other hand, physical meanings of the mean ergodic theorem can be explained as follows. We now turn to one-parameter flow of transformations. In order to study continuous averages

$$\frac{1}{t} \int_0^t f(F_s x) ds$$

fix some $s_0 \in \mathbb{R}$ and consider the averages of the form

$$\frac{1}{N} \sum_{n=0}^{N-1} f(T^n x)$$

where $T = F_{s_0}$. In reality, the measurements can be done only approximately at times $t = 0, 1, \dots, N-1$, and it is natural to consider the perturbed averages

$$\frac{1}{N} \sum_{n=0}^{N-1} f(T^{n+\delta_n}x)$$

where $\{\delta_n\}_{n \in \mathbb{N}}$ is an independent random sequence in a small interval $(-\epsilon, \epsilon)$. Assuming that $T = F_{s_0}$ is ergodic, we would like to know whether for large N , the averages

$$\frac{1}{N} \sum_{n=0}^{N-1} f(T^{n+\delta_n}x)$$

are close to

$$\int_X f(x) d\mu(x)$$

The answer to this question is satisfactory if one is concerned with norm convergence (see, e.g., Bergelson *et al.* (1994)).

Induced Transformations and Tower Constructions

Suppose T is a measure-preserving transformation on a probability space (X, \mathcal{B}, μ) and $A \in \mathcal{B}$ with $\mu(A) > 0$. Let us transform A into a space with normalized measure by choosing the σ -algebra \mathcal{B}_A consisting of all subsets $E \subset A, E \in \mathcal{B}$ and setting $\mu_A(E) = \mu(A \cap E)/\mu(A)$. Let $R_A: A \rightarrow \mathbb{N} \cup \{\infty\}$ be the “first return function,” that is, $R_A(x) := \inf\{n \in \mathbb{N} \mid T^n x \in A\}$. Then it follows from the Poincaré recurrence theorem that $\mu_A(\{x \in A \mid R_A(x) < \infty\}) = 1$. Define $T_A: \{x \in A \mid R_A(x) < \infty\} \rightarrow A$ by $T_A x := T^{R_A(x)} x$, which is called the “induced transformation” over A (constructed from T). For each $n \in \mathbb{N}$ we define $A_n := \{x \in A \mid R_A(x) = n\}$. Then for every $E \in \mathcal{B}_A$ we see that $T_A^{-1}E = \bigcup_{n=1}^{\infty} T^{-n}(A_n \cap E)$. Hence, if T is invertible, then we have immediately $\mu_A(T_A^{-1}E) = \mu_A(E)$; thus, μ_A is invariant under T_A . Even if T is noninvertible, since for every $k \geq 1$ the equality,

$$\begin{aligned} & \mu\left(\bigcup_{j=0}^{k-1} T^{-j} A^c \cap T^{-k}(A \cap E)\right) \\ &= \mu(A_{k+1} \cap T^{-(k+1)}E) \\ &+ \mu\left(\bigcup_{j=0}^k T^{-j} A^c \cap T^{-(k+1)}(A \cap E)\right) \end{aligned}$$

holds, we have $\mu(E) = \sum_{k=1}^{\infty} \mu(A_k \cap T^{-k}E) = \mu(T_A^{-1}E)$, which allows us to see that T_A preserves μ_A . We note that for every $E \in \mathcal{B}_A$ with $\mu(E) > 0$,

$\{n \in \mathbb{N} \mid T^n x \in E\} = \{n \in \mathbb{N} \mid T_A^n x \in E\}$. Therefore, for a.e. $x \in E$, $\sum_{n=1}^{\infty} 1_E T^n(x) = \sum_{n=1}^{\infty} 1_E T_A^n(x)$. This equality allows us to see that if (T, μ) is ergodic then (T_A, μ_A) is ergodic. Indeed, suppose $T_A^{-1}E = E$ and $\mu(A \cap E^c) > 0$. Then for $x \in A \cap E^c$, we have $\sum_{n=1}^{\infty} 1_E T_A^n(x) = 0$. On the other hand, as $E \subset \bigcup_{n=1}^{\infty} T^{-n}E \pmod{\mu}$, $\bigcup_{n=1}^{\infty} T^{-n}E = \bigcup_{n=0}^{\infty} T^{-n}E$ is a T -invariant set. Hence, ergodicity of (T, μ) allows us to see that $\bigcup_{n=1}^{\infty} T^{-n}E = X \pmod{0}$, which implies $\sum_{n=1}^{\infty} 1_E T^n(x) = \infty$. In the case when T is invertible, we can write $\int_A R_A d\mu = \mu(\bigcup_{n \geq 0} T^n A)$, so that Kac's formula (Darling and Kac 1957):

$$\int_A R_A d\mu_A = \mu(A)^{-1}$$

is valid when $\bigcup_{n \geq 0} T^n A = X \pmod{\mu}$. In particular, $\mu(\bigcup_{n \geq 0} T^n A) = 1$ if T is ergodic. The key to establish the Kac formula is to show that $T^i A_k (0 \leq i \leq k-1, k \geq 1)$ are pairwise disjoint. This property holds when T is invertible. On the other hand, in the case when T is noninvertible, if $\bigcup_{n=0}^{\infty} T^{-n} A = X \pmod{0}$ then we can establish, for every $E \in \mathcal{B}$,

$$\mu(E) = \mu(A) \int_A \sum_{b=0}^{R_A(x)-1} 1_E T^b(x) d\mu_A(x) \quad [1]$$

by noting that the following equality holds for all $n \geq 1$:

$$\begin{aligned} \mu(E) &= \sum_{k=1}^n \mu_A\left(A \cap \bigcap_{b=1}^k T^{-b} A^c \cap T^{-k} A\right) \\ &+ \mu_A(A \cap E) + \mu\left(\left(\bigcup_{j=0}^n T^{-j} A\right)^c \cap T^{-n} E\right) \end{aligned}$$

Then choosing $E = X$ allows one to establish the Kac formula. As we have observed in the above, the assumption that $\bigcup_{n=0}^{\infty} T^{-n} A = X \pmod{0}$ is automatically satisfied if (T, μ) is ergodic. Conversely, if (T_A, μ_A) is ergodic and $\bigcup_{n=1}^{\infty} T^{-n} A \pmod{\mu}$ holds, then (T, μ) is ergodic. We should remark that the formula [1] allows one to obtain a T -invariant measure when a T_A -invariant measure μ_A is obtained previously. Even if R_A is nonintegrable, we may have a σ -finite infinite invariant measure. Then if μ_A is ergodic, μ obtained by [1] is still ergodic (i.e., $T^{-1}E = E$ implies that $\mu(E) = 0$ or $\mu(E^c) = 0$) under the assumption that $\bigcup_{n=1}^{\infty} T^{-n} A = X \pmod{\mu}$ (cf. Aaronson (1997)). In particular, the recent progress in the study of nonhyperbolic systems strongly depends on such constructions of induced maps over hyperbolic regions. More specifically, if one can find a subset A over which the induced map possesses an

invariant measure satisfying nice statistical properties, then the formula [1] may give a σ -finite invariant measure μ for the original map T which reflects the statistical properties of the induced system. The fundamental problem in the study of nonhyperbolic phenomena arising from complex systems is to clarify how to predict statistical properties of nonhyperbolic systems (T, μ) by using those of induced systems (T_A, μ_A) over hyperbolic regions. We should claim that induced maps are well defined over positive-measure sets with respect to a reference measure ν that is "conservative." Here conservativity of (T, ν) implies that there are no wandering sets of positive measure with respect to ν . In many cases, the reference measures are physical measures (e.g., Lebesgue measures, conformal measures) which satisfy nonsingularity with respect to T . Here nonsingularity of ν means that $\nu T^{-1} \sim \nu$. Then as long as we obtain a T_A -invariant measure μ_A which is equivalent to $\nu|_A$, the formula [1] may give us a T -invariant σ -finite measure which is equivalent to ν .

At the end of this section, we will explain that the formula [1] can be obtained via Rohlin tower (Kakutani's skyscraper) in the case when T is invertible. This tower construction is a dual construction to the construction of induced transformations. Assuming that we are given an invertible transformation T of the measure space (X, \mathcal{B}, μ) , consider the measurable integer-valued positive function $f \in L^1(X, \mathcal{B}, \mu)$. By using this function, construct a new measure space X^f , whose points are of the form (x, i) , where $x \in X$, $1 \leq i \leq f(x)$ and i is an integer. The σ -algebra \mathcal{B}^f of measurable sets in X^f is constructed in an obvious way. The measure μ^f is defined as follows: for any subset of the form (A, i) , $A \in \mathcal{B}$ we put

$$\mu^f((A, i)) := \frac{\mu(A)}{\int_X f d\mu}$$

Let

$$T^f(x, i) = \begin{cases} (x, i+1) & \text{if } i+1 \leq f(x) \\ (Tx, 1) & \text{if } i+1 > f(x) \end{cases}$$

It is easy to see that T^f preserves μ^f . The space can naturally be visualized as a tower whose foundation is the space X and which has $f(x)$ floors over the point $x \in X$. The space X is identified with the set of points $(x, 1)$. We see that $T = (T^f)_X$ and the construction of (X^f, T^f) is called the Rohlin tower over X . Let T be an invertible measure-preserving transformation on a probability space (X, \mathcal{B}, μ) and $A \in \mathcal{B}$ with $\mu(A) > 0$. Suppose that

$X = \bigcup_{n=0}^{\infty} T^n A \pmod{\mu}$. Then T is represented as the Rohlin tower $(A^{R_A}, \mathcal{B}^{R_A}, (\mu_A)^{R_A})$ over A as follows. We define $p: (A^{R_A}, \mathcal{B}^{R_A}, (\mu_A)^{R_A}) \rightarrow (X, \mathcal{B}, \mu)$ by $p(x, i) := T^i x$. Then p is an isomorphism satisfying $p(T^{R_A})_A = Tp$ (almost everywhere). Moreover, we can verify that $(\mu_A)^{R_A} p^{-1} = \mu$ by assuming ergodicity of μ . This is because $\forall E \in \mathcal{B}$ we have

$$\begin{aligned} \left(\bigcup_{n=0}^{\infty} T^n A \right) \cap E \\ = \bigcup_{n=1}^{\infty} \bigcup_{i=0}^{n-1} p((A_n \cap T^{-i} E) \times \{i\}) \end{aligned}$$

so that

$$\begin{aligned} (\mu_A)^{R_A}(p^{-1}E) &= \sum_{n=1}^{\infty} \sum_{i=0}^{n-1} \frac{\mu_A(A_n \cap T^{-i} E)}{\int_A R_A d\mu_A} \\ &= \mu(A) \int_A \sum_{h=0}^{R_A(x)-1} 1_E T^h(x) d\mu_A(x) \end{aligned}$$

On the other hand, in the case when T is noninvertible, the formula [1] is not necessarily obtained by any tower construction, except in very special cases. For example, even if T is not invertible, the tower construction is valid if $T|_A$ and $T|_{A^c}$ are one-to-one and $TA = X$.

Convergence to Equilibrium States and Mixing Properties

Let $T: X \rightarrow X$ be a measure-preserving transformation on a probability space (X, \mathcal{B}, μ) . We call T to be "weak mixing" if for any $A, B \in \mathcal{B}$

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=0}^{N-1} \left| \mu(T^{-n}A \cap B) - \mu(A)\mu(B) \right| = 0$$

The weak-mixing property of (T, μ) can be represented by; $\forall f, g \in L^2(X, \mathcal{B}, \mu)$

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=0}^{N-1} \left| \int_X (f T^n) g d\mu - \int_X f d\mu \int_X g d\mu \right| = 0$$

and this is equivalent to the ergodicity of $(T \times T, \mu \times \mu)$. Moreover, (T, μ) is weak mixing if and only if the unitary operator $U: \mathcal{H} \rightarrow \mathcal{H}$ defined by $Uf(x) = f(Tx)$ has no eigenfunctions that are not constants ($\mu \bmod 0$). We say that the operator U has continuous spectrum if there are no eigenvectors. If \mathcal{H} is the closure of the linear span of the eigenvectors, then we say that the operator U has pure point spectrum. The weak-mixing property of (T, μ) just implies that U restricted on the orthogonal subspace of the subspace consisting of

constant functions has continuous spectrum. We recall that if U has one as a simple eigenvalue then T is ergodic. Additionally, if there are no other eigenvalues, then T is weakly mixing. Hence, if T is weak mixing, then it is necessarily ergodic. The next property corresponds to the term “relaxation” in physics literature which is used to describe processes under which the system passes to a certain stationary state independently of its original state. We call T (strong) mixing if for any $A, B \in \mathcal{B}$

$$\lim_{n \rightarrow \infty} \mu(T^{-n}A \cap B) = \mu(A)\mu(B)$$

Then (T, μ) is (strong) mixing if and only if for any $f, g \in L^2(X, \mathcal{B}, \mu)$

$$\lim_{n \rightarrow \infty} \int_X (fT^n)g \, d\mu = \int_X f \, d\mu \int_X g \, d\mu$$

and mixing is necessarily weak mixing. Moreover, for any probability measure ν absolutely continuous with respect to μ , one can show that $\lim_{n \rightarrow \infty} \nu(T^{-n}A) = \mu(A)$ for every $A \in \mathcal{B}$. Thus, any nonequilibrium distribution tends to an equilibrium one with time. The mixing property has a significant meaning from a physical point of view, as it implies decay of correlation of observable functions; moreover, limiting distributions of averaged observables are determined by the decay rates of correlation functions for many cases (e.g., hyperbolic systems). For any $f \in L^2(X, \mathcal{B}, \mu)$ we consider the scalar products $s_n = s_n(f) = (U^n f, f)$, $n \geq 0$ and define $s_n := \bar{s}_{-n}$ for $n < 0$. The sequence $\{s_n\}_{n \in \mathbb{Z}}$ is positive definite and so by Bochner's theorem, we can write $s_n(f) = \int_0^1 \exp[2\pi i n \lambda] d\sigma_f(\lambda)$, where σ_f is a finite Borel measure on the unit circle S^1 and satisfies the condition that $\sigma_f(S^1) = \|f\|^2$. Such a measure is called a spectral measure of f . We see that T is mixing iff for any $f \in L^2(X, \mathcal{B}, \mu)$ with $\int_X f \, d\mu = 0$ the Fourier coefficients $\{s_n\}$ of the spectral measure σ_f tend to zero as $|n| \rightarrow \infty$. Let (X, \mathcal{B}, μ) be isomorphic to $([0, 1], \mathcal{B}_0, \lambda)$, where \mathcal{B}_0 is the Borel σ -algebra on $[0, 1]$ and λ is the normalized Lebesgue measure of $[0, 1]$. Then we call a measure-preserving transformation T on (X, \mathcal{B}, μ) an exact endomorphism if $\bigcap_{n=0}^{\infty} T^{-n}\mathcal{B} = \{X, \emptyset\} (\mu \bmod 0)$. We can verify that an exact endomorphism is (strong) mixing (Rohlin 1964). Moreover, μ is exact if for any positive-measure set $A \in \mathcal{B}$ with $T^n A \in \mathcal{B} (\forall n \geq 0)$ $\lim_{n \rightarrow \infty} \mu(T^n A) = 1$ holds. Let T be a nonsingular transformation on (X, \mathcal{B}, ν) , that is, $\nu T^{-1} \sim \nu$. Then we can define the transfer (Perron–Frobenius) operator $\mathcal{L}_\nu : L^1(X, \nu) \rightarrow L^1(X, \nu)$ by $\mathcal{L}_\nu f := d(f\nu)T^{-1}/d\nu$, which satisfies

$$\int_X (\mathcal{L}_\nu f)g \, d\nu = \int_X f(gT) \, d\nu \quad (\forall g \in L^\infty(X, \nu))$$

We say that a nonsingular measure ν is exact if $A \in \bigcap_{n=0}^{\infty} T^{-n}\mathcal{B}$ implies $\nu(A)\nu(A^c) = 0$. By Lin's theorem (Lin 1971) the exactness of ν can be described as follows; $\forall f \in L^1(X, \nu)$ with $\int_X f \, d\nu = 0$, $\lim_{n \rightarrow \infty} \|\mathcal{L}_\nu^n f\|_1 = 0$. Let $\mu = h\nu$ be an exact T -invariant probability measure equivalent to ν . Then the upper bounds of mixing rates of the exact measure $\mu = h\nu$ are determined by the speed of L^1 -convergence of the iterated transfer operators $\{\mathcal{L}_\nu^n\}$. This is because $\mathcal{L}_\nu h = h$ and for every $f \in L^1(X, \nu)$ with $\int_X f \, d\nu = 1$, $\lim_{n \rightarrow \infty} \|\mathcal{L}_\nu^n f - h\|_1 = 0$. Hence, the property $\mathcal{L}_\mu f = h^{-1}\mathcal{L}_\nu(hf)$ allows one to see that for every $f, g \in L^\infty(X, \mu)$ the correlation function

$$C_{f,g}(n) := \left| \int_X (fT^n)g \, d\mu - \int_X f \, d\mu \int_X g \, d\mu \right|$$

is bounded from above by

$$\begin{aligned} & \|f\|_\infty \|\mathcal{L}_\mu^n g - \int_X g \, d\mu\|_1 \\ &= \|f\|_\infty \|h^{-1}\{\mathcal{L}_\nu^n(gh) - P(gh)\}\|_1 \end{aligned}$$

where $P : L^1(X, \nu) \rightarrow L^1(X, \nu)$ is a linear operator defined by $Pf := h \int_X f \, d\nu$. The operator P is the one-dimensional projection operator associated to the eigenvalue 1 (which is maximal in many cases) of \mathcal{L}_ν satisfying $P^2 = P$ and $P\mathcal{L}_\nu = \mathcal{L}_\nu P = P$. Moreover, since $\mathcal{L}_\nu^n - P = (\mathcal{L}_\nu - P)^n$, the exponential decay of mixing rates follows from the spectral gap of \mathcal{L}_ν , that is, 1 is the simple isolated maximal eigenvalue of \mathcal{L}_ν .

Entropy and Reversibility

We recall one of the fundamental problems of ergodic theory, namely deciding when two automorphisms T_1, T_2 of probability spaces $(X_1, \mathcal{B}_1, \mu_1)$ and $(X_2, \mathcal{B}_2, \mu_2)$ are equivalent. The approach developed for this problem involved the study of spectral properties of the associated isometric operators $U_i : L^2(X_i, \mu_i) \rightarrow L^2(X_i, \mu_i) (i=1, 2)$ and is based on the concept of the entropy of automorphism T , introduced by Kolmogorov (1958). The entropy is a non-negative number, which is the same for equivalent automorphisms. For example, the entropy of the Bernoulli shift $\sigma : \Pi_{n \in \mathbb{Z}}\{1, 2, \dots, d\} \rightarrow \Pi_{n \in \mathbb{Z}}\{1, 2, \dots, d\}$ with probability vector (p_1, p_2, \dots, p_d) is equal to $-\sum_{k=1}^d p_k \log p_k$. A remarkable theorem of Ornstein (1970) states that Bernoulli shifts with the same entropy are equivalent. On the other hand, Shannon (1948) introduced a notion of entropy in his work information theory, which is essentially the same as Kolmogorov's. Let $T : X \rightarrow X$ be a measure-preserving transformation on a probability space (X, \mathcal{B}, μ) . We define the entropy of a measurable partition α of X by

$H_\mu(\alpha) = -\sum_{A \in \mathcal{A}} \mu(A) \log \mu(A)$ and define the entropy of T with respect to α by

$$h_\mu(T, \alpha) := \lim_{n \rightarrow \infty} \frac{1}{n} H_\mu \left(\bigvee_{i=0}^{n-1} T^{-i} \alpha \right)$$

Then the (measure-theoretic) entropy of T is defined by

$$h_\mu(T) = \sup_{\alpha: H_\mu(\alpha) < \infty} h_\mu(T, \alpha)$$

The next Abramov theorem gives an important method of practical computation: let $\{\alpha_n\}_{n \geq 1}$ be an increasing sequence of partitions with $H_\mu(\alpha_n) < \infty$ ($\forall n \geq 1$) and such that $\bigcup_{n \geq 1} \alpha_n$ generates the σ -algebra \mathcal{B} . Then $h_\mu(T) = \lim_{n \rightarrow \infty} h_\mu(T, \alpha_n)$. We say that a partition α is called a generator for a noninvertible measure-preserving transformation T on a probability space (X, \mathcal{B}, μ) if $\bigvee_{i=0}^{\infty} T^{-i} \alpha$ generates \mathcal{B} . If T is invertible then a partition α is called a generator if $\bigvee_{i=-\infty}^{\infty} T^{-i} \alpha$ generates \mathcal{B} . In the case when α is a generator with $H_\mu(\alpha) < \infty$, by the Kolmogorov–Sinai theorem we have $h_\mu(T) = h_\mu(T, \alpha)$. Let $\alpha_n(x)$ denote an element of $\bigvee_{i=0}^{n-1} T^{-i} \alpha$ containing $x \in X$. By the Shannon–McMillan–Breiman theorem, if T is a measure-preserving transformation of the probability space (X, \mathcal{B}, μ) and α is a partition of X with $H_\mu(\alpha) < \infty$, then $-(1/n) \mu(\alpha_n(x))$ converges μ -a.e. and in $L^1(X, \mu)$ as $n \rightarrow \infty$. If T is ergodic, then the limit coincides with $h_\mu(T, \alpha)$. Now we can apply these results to piecewise expanding transitive (countable) Markov transformations T of $X \subset \mathbb{R}^d$. More specifically, let ν be the normalized Lebesgue measure of X . It is well known that under certain conditions there exists the unique ergodic invariant probability measure μ equivalent to ν . Then we can establish the Rohlin's entropy formula (Rohlin 1964):

$$h_\mu(T) = \int_X \log |\det DT| d\mu$$

under the assumptions that $H_\nu(\alpha) < \infty$ and $\log |\det DT| \in L^1(X, \nu)$. In particular, if α is a finite partition and $\phi = -\log |\det DT|$ is piecewise Hölder continuous, then the entropy formula just implies that μ is an equilibrium state for the potential ϕ in the following sense:

$$h_\mu(T) + \int_X \phi d\mu = \sup \{ h_m(T) + \int_X \phi dm \mid m$$

is a T -invariant Borel probability measure on X }, where the right-hand side is called the pressure for ϕ (Walters 1981).

We now turn our attention to results which relate entropy to Lyapunov exponent in the context of smooth invertible systems. Let T be a diffeomorphism of a compact manifold M . We say that $x \in M$ is a regular

point of T if there exist numbers $\lambda_1(x) > \lambda_2(x) > \dots > \lambda_d(x)$ and a decomposition $T_x M = E_1(x) + E_2(x) + \dots + E_d(x)$ such that

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log \|DT^n(x)u\| = \lambda_j(x)$$

for every $0 \neq u \in E_j(x)$ and every $1 \leq j \leq d$. Let Λ be the set of regular points of T . Then we define a function

$$\chi(x) := \sum_{\lambda_j(x) \geq 0} \lambda_j(x) \dim E_j(x)$$

In the case when all Lyapunov exponents at x are negative, we put $\chi(x) = 0$. Then for every T -invariant Borel probability measure μ on (X, \mathcal{B}) , it holds that $h_\mu(T) \leq \int_X \chi d\mu$ (Ruelle 1978). Moreover, the equality holds whenever T is C^1 -Hölder and μ is absolutely continuous with respect to the Lebesgue measure of X (Pesin 1977). Let T be a transitive C^1 -Hölder Anosov diffeomorphism. E^s, E^u denote the stable and unstable fiber bundles of T . Suppose that μ_+ is the unique T -invariant probability measure which satisfies

$$\int_M f d\mu_+ = \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{k=0}^{n-1} \int_M f T^k(x)$$

for every continuous function $f: M \rightarrow \mathbb{R}$ and almost everywhere $x \in M$ with respect to the Lebesgue measure. The probability measure is the so-called Sinai–Ruelle–Bowen (SRB) measure. Then we have

$$h_{\mu_+}(T) = \int_M \log |\det DT(x)|_{E_x^u} d\mu_+(x)$$

On the other hand, we have

$$\begin{aligned} h_{\mu_+}(T) &= \int_M \log |\det DT^{-1}(x)|_{E_x^s} d\mu_+(x) \\ &\quad + \int_M \log |\det DT(x)| d\mu_+(x) \end{aligned}$$

We also define anti-SRB measure μ_- by replacing T by T^{-1} . Then the SRB measure μ_+ is absolutely continuous with respect to the Lebesgue measure of M iff μ_+ coincides with the anti-SRB measure μ_- (Bowen 1975). Hence, the SRB measure is absolutely continuous iff $\int_M \log |\det DT(x)| d\mu_+(x) = 0$. This property is sometimes explained as “zero entropy production” and also as “reversibility” in the context of non-equilibrium statistical mechanics (Ruelle 1997).

See also: Chaos and Attractors; Determinantal Random Fields; Dissipative Dynamical Systems of Infinite Dimension; Dynamical Systems and Thermodynamics; Finitely Correlated States; Fourier Law; Fractal Dimensions in Dynamics; Homeomorphisms and Diffeomorphisms of the Circle; Hyperbolic Billiards; Hyperbolic dynamical Systems; Intermittency in

Turbulence; Large Deviations in Equilibrium Statistical Mechanics; Lyapunov Exponents and Strange Attractors; Nonequilibrium Statistical Mechanics: Interaction Between Theory and Numerical Simulations; Nonequilibrium Statistical Mechanics (Stationary): Overview; Phase Transitions in Continuous Systems; Polygonal Billiards; Regularization for Dynamical Zeta Functions; Singularity and Bifurcation Theory; von Neumann Algebras: Introduction, Modular Theory, and Classification Theory.

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Euclidean Field Theory

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Introduction

In this article, we consider Euclidean field theory as a formulation of quantum field theory which lives in some Euclidean space, and is expressed in probabilistic terms. Methods arising from Euclidean field theory have been introduced in a very successful way in the study of concrete models of constructive quantum field theory.

Euclidean field theory was initiated by Schwinger (1958) and Nakano (1959), who proposed to study the vacuum expectation values of field products analytically continued into the Euclidean region (Schwinger functions), where the first three (spatial) coordinates of a world point are real and the last one (time) is purely imaginary (Schwinger points). The

possibility of introducing Schwinger functions, and their invariance under the Euclidean group are immediate consequences of the now classic formulation of quantum field theory in terms of vacuum expectation values given by Wightman (Streater and Wightman 1964). The convenience of dealing with the Euclidean group, with its positive-definite scalar product, instead of the Lorentz group, is evident, and has been exploited by several authors, in different contexts.

The next step was made by Symanzik (1966), who realized that Schwinger functions for boson fields have a remarkable positivity property, allowing to introduce Euclidean fields on their own sake. Symanzik also pointed out an analogy between Euclidean field theory and classical statistical mechanics, at least for some interactions (Symanzik 1969).

This analogy was successfully extended, with a different interpretation, to all boson interactions by Guerra *et al.* (1975), with the purpose of using rigorous results of modern statistical mechanics for

the study of constructive quantum field theory, within the program advocated by Wightman (1967), and further pursued by Glimm and Jaffe (see Glimm and Jaffe (1981) for an overall presentation).

The most dramatic advance of Euclidean theory was due to Nelson (1973a, b). He was able to isolate a crucial property of Euclidean fields (the Markov property) and gave a set of conditions for these fields, which allow us to derive all properties of relativistic quantum fields satisfying Wightman axioms. The Nelson theory is very deep and rich in new ideas. Even after so many years since the basic papers were published, we lack a complete understanding of the radical departure from the conventional theory afforded by Nelson's ideas, especially about their possible further developments.

By using the Nelson scheme, in particular a very peculiar symmetry property, it was very easy to prove (Guerra 1972) the convergence of the ground-state energy density, and the van Hove phenomenon in the infinite-volume limit for two-dimensional boson theories. A subsequent analysis (Guerra *et al.* 1972) gave other properties of the infinite-volume limit of the theory, and allowed a remarkable simplification in the proof of a very important regularity property for fields, previously established by Glimm and Jaffe.

Since then, all work on constructive quantum field theory has exploited in different ways ideas coming from Euclidean field theory. Moreover, a very important reconstruction theorem has been established by Osterwalder and Schrader (1973), allowing a reconstruction of relativistic quantum fields from the Euclidean Schwinger functions, and avoiding the previously mentioned Nelson reconstruction theorem, which is technically more difficult to handle.

This article is intended to be an introduction to the general structure of Euclidean quantum field theory, and to some of the applications to constructive quantum field theory. Our purpose is to show that, 50 years after its introduction, the Euclidean theory is still interesting, both from the point of view of technical applications and physical interpretation.

The article is organized as follows. In the next section, by considering simple systems made of a single spinless relativistic particle, we introduce the relevant structures in both Euclidean and Minkowski worlds. In particular, a kind of (pre)Markov property is introduced already at the one-particle level.

Next we present a description of the procedure of second quantization on the one-particle structure. The free Markov field is introduced, and its crucial Markov property explained. Following Nelson, we use probabilistic concepts and methods, whose relevance for constructive quantum field theory became immediately more and more apparent. The

very structure of classical statistical mechanics for Euclidean fields is firmly based on these probabilistic methods. This is followed by an introduction of interaction, and we show the connection between the Markov theory and the Hamiltonian theory, for two-dimensional space-cutoff interacting scalar fields. In particular, we present the Feynman–Kac–Nelson formula that gives an explicit expression of the semigroup generated by the space-cutoff Hamiltonian in Φ_{OK} space. We also deal with some applications to constructive quantum field theory. This is followed by a short discussion about the physical interpretation of the theory. In particular, we discuss the Osterwalder–Schrader reconstruction theorem on Euclidean Schwinger functions, and the Nelson reconstruction theorem on Euclidean fields. For the sake of completeness, we sketch the main ideas of a proposal, advanced in Guerra and Ruggiero (1973), according to which the Euclidean field theory can be interpreted as a stochastic field theory in the physical Minkowski spacetime.

Our treatment will be as simple as possible, by relying on the basic structural properties, and by describing methods of presumably very long lasting power. The emphasis given to probabilistic methods, and to the statistical mechanics analogy, is a result of the historical development. Our opinion is that not all possibilities of Euclidean field theory have been fully exploited yet, both from technical and physical points of view.

One-Particle Systems

A system made of only one relativistic scalar particle, of mass $m > 0$, has a quantum state space represented by the positive-frequency solutions of the Klein–Gordon equation. In momentum space, with points $p_\mu, \mu = 0, 1, 2, 3$, let us introduce the upper mass hyperboloid, characterized by the constraints $p^2 \equiv p_0^2 - \sum_{i=1}^3 p_i^2 = m^2, p_0 \geq m$, and the relativistic invariant measure on it, formally given by $d\mu(p) = \theta(p_0) \delta(p^2 - m^2) dp$, where θ is the step function $\theta(x) = 1$ if $x \geq 0$, and $\theta(x) = 0$ otherwise, and dp is the four-dimensional Lebesgue measure. The Hilbert space of quantum states F is given by the square-integrable functions on the mass hyperboloid equipped with the invariant measure $d\mu(p)$. Since in some reference frame the mass hyperboloid is uniquely characterized by the space values of the momentum \underline{p} , with the energy given by $p_0 \equiv \omega(\underline{p}) = \sqrt{\underline{p}^2 + m^2}$, the Hilbert space F of the states is, in fact, made of those complex-valued tempered distributions f in the configuration space R^3 whose Fourier transforms, $\hat{f}(\underline{p})$, are square-integrable functions in momentum space with respect to the image of the relativistic invariant measure $dp/2\omega(\underline{p})$, where

$d\mathbf{p}$ is the Lebesgue measure in momentum space. The scalar product on F is defined by

$$\langle f, g \rangle_F = (2\pi)^3 \int \tilde{f}^*(\mathbf{p}) \tilde{g}(\mathbf{p}) \frac{d\mathbf{p}}{2\omega(\mathbf{p})}$$

where we have normalized the Fourier transform in such a way that

$$\begin{aligned} f(\mathbf{x}) &= \int \exp(i\mathbf{p} \cdot \mathbf{x}) \tilde{f}(\mathbf{p}) d\mathbf{p} \\ \tilde{f}(\mathbf{p}) &= (2\pi)^{-3} \int \exp(-i\mathbf{p} \cdot \mathbf{x}) \tilde{f}(\mathbf{x}) d\mathbf{x} \\ \int \exp(i\mathbf{p} \cdot \mathbf{x}) d\mathbf{p} &= (2\pi)^3 \delta(\mathbf{x}) \end{aligned}$$

The scalar product on F can also be expressed in the form

$$\langle f, g \rangle_F = \iint f(\mathbf{x}')^* W(\mathbf{x}' - \mathbf{x}) g(\mathbf{x}) d\mathbf{x}' d\mathbf{x}$$

where we have introduced the two-point Wightman function at fixed time, defined by

$$W(\mathbf{x}' - \mathbf{x}) = (2\pi)^{-3} \int \exp(i\mathbf{p} \cdot (\mathbf{x}' - \mathbf{x})) \frac{d\mathbf{p}}{2\omega(\mathbf{p})}$$

A unitary irreducible representation of the Poincaré group can be defined on F in the obvious way. In particular, the generators of space translations are given by multiplication by the components of \mathbf{p} in momentum space, and the generator of time translations (the energy of the particle) is given by $\omega(\mathbf{p})$.

For the scalar product of time-evolved wave functions, we can write

$$\begin{aligned} &\langle \exp(-it')f, \exp(-it)g \rangle_F \\ &= \iint f(\mathbf{x}')^* W(t' - t, \mathbf{x}' - \mathbf{x}) g(\mathbf{x}) d\mathbf{x}' d\mathbf{x} \end{aligned}$$

where we have introduced the two-point Wightman function, defined by

$$\begin{aligned} &W(t' - t, \mathbf{x}' - \mathbf{x}) \\ &= (2\pi)^{-3} \int \exp(-i(t - t')) \exp(i\mathbf{p} \cdot (\mathbf{x}' - \mathbf{x})) \frac{d\mathbf{p}}{2\omega(\mathbf{p})} \end{aligned}$$

To the physical single-particle system living in Minkowski spacetime, we associate a kind of mathematical image, living in Euclidean space, from which all properties of the physical system can be easily derived. We start from the two-point Schwinger function

$$S(\mathbf{x}) = \frac{1}{(2\pi)^4} \int \frac{\exp(i\mathbf{p} \cdot \mathbf{x})}{\sqrt{p^2 + m^2}} d\mathbf{p}$$

which is the analytic continuation of the previously given two-point Wightman function into the Schwinger

points. Here $\mathbf{x}, \mathbf{p} \in R^4$, and $\mathbf{p} \cdot \mathbf{x} = \sum_{i=1}^4 x_i p_i$. Here $d\mathbf{p}$ and $d\mathbf{x}$ are the Lebesgue measures in the R^4 momentum and configuration spaces, respectively. The function $S(\mathbf{x})$ is positive and analytic for $\mathbf{x} \neq 0$, decreases as $\exp(-m\|\mathbf{x}\|)$ as $\mathbf{x} \rightarrow \infty$, and satisfies the equation

$$(-\Delta + m^2)S(\mathbf{x}) = \delta(\mathbf{x})$$

where $\Delta = \sum_{i=1}^4 \partial^2 / \partial x_i^2$ is the Laplacian in four dimensions.

The mathematical image we are looking for is described by the Hilbert space N of those tempered distributions in four-dimensional configuration space R^4 whose Fourier transforms are square integrable with respect to the measure $d\mathbf{p} / \sqrt{p^2 + m^2}$. The scalar product on N is defined by

$$\langle f, g \rangle_N = (2\pi)^4 \int \tilde{f}^*(\mathbf{p}) \tilde{g}(\mathbf{p}) \frac{d\mathbf{p}}{\sqrt{p^2 + m^2}}$$

Four-dimensional Fourier transforms are normalized as follows:

$$\begin{aligned} f(\mathbf{x}) &= \int \exp(i\mathbf{p} \cdot \mathbf{x}) \tilde{f}(\mathbf{p}) d\mathbf{p} \\ \tilde{f}(\mathbf{p}) &= (2\pi)^{-4} \int \exp(-i\mathbf{p} \cdot \mathbf{x}) \tilde{f}(\mathbf{x}) d\mathbf{x} \\ \int \exp(i\mathbf{p} \cdot \mathbf{x}) d\mathbf{p} &= (2\pi)^4 \delta(\mathbf{x}) \end{aligned}$$

We also write

$$\begin{aligned} \langle f, g \rangle_N &= \iint f^*(\mathbf{x}) S(\mathbf{x} - \mathbf{y}) g(\mathbf{y}) d\mathbf{x} d\mathbf{y} \\ &= \langle f, (-\Delta + m^2)^{-1} g \rangle \end{aligned}$$

where \langle, \rangle is the ordinary Lebesgue product defined on Fourier transforms and, in momentum space, $(-\Delta + m^2)^{-1}$ amounts to a multiplication by $(p^2 + m^2)^{-1}$. The Schwinger function $S(\mathbf{x} - \mathbf{y})$ is formally the kernel of the operator $(-\Delta + m^2)^{-1}$. The Hilbert space N is the carrier space of a unitary (nonirreducible) representation of the four-dimensional Euclidean group $E(4)$. In fact, let (a, R) be an element of $E(4)$

$$\begin{aligned} (a, R) : R^4 &\rightarrow R^4 \\ x &\rightarrow Rx + a \end{aligned}$$

where $a \in R^4$, and R is an orthogonal matrix, $RR^T = R^T R = 1_4$. Then the transformation $u(a, R)$ defined by

$$\begin{aligned} u(a, R) : N &\rightarrow N \\ f(\mathbf{x}) &\rightarrow (u(a, R)f)(\mathbf{x}) = f(R^{-1}(\mathbf{x} - a)) \end{aligned}$$

provides the representation. In particular, we consider the reflection r_0 with respect to the hyperplane

$x_4=0$, and the translations $u(t)$ in the x_4 -direction. Then we have $r_0 u(t) r_0 = u(-t)$, and analogously for other hyperplanes.

Now we introduce a local structure on N by considering, for any closed region A of R^4 , the subspace N_A of N made by distributions in N with support on A . We call e_A the orthogonal projection on N_A . It is obvious that if $A \in B$ then $N_A \in N_B$ and $e_A e_B = e_B e_A = e_A$. A kind of (pre)Markov property for one-particle systems is introduced as follows. Consider a closed three-dimensional piecewise smooth manifold σ , which divides R^4 in two closed regions A and B , having σ in common. Therefore, $\sigma \in A, \sigma \in B, A \cap B = \sigma, A \cup B = R^4$. Let N_A, N_B, N_σ , and e_A, e_B, e_σ be the associated subspaces and projections, respectively. Then $N_\sigma \subset N_A, N_\sigma \subset N_B$, and $e_\sigma e_A = e_A e_\sigma = e_\sigma, e_\sigma e_B = e_B e_\sigma = e_\sigma$. It is very simple to prove the following:

Theorem 1 *Let e_A, e_B, e_σ be defined as above, then $e_A e_B = e_B e_A = e_\sigma$.*

Clearly, it is enough to show that for any $f \in N$ we have $e_A e_B f \in N_\sigma$. In that case, $e_\sigma e_A e_B f = e_A e_B f$, from which the theorem easily follows. Since $e_A e_B f$ has support on A , we must show that for any C_0^∞ function g with support on A_σ we have $\langle g, e_A e_B f \rangle = 0$. Then $e_A e_B f$ has support on σ , and the proof is complete. Now we have

$$\begin{aligned} \langle g, e_A e_B f \rangle &= \langle (-\Delta + m^2)g, e_A e_B f \rangle_N \\ &= \langle e_A (-\Delta + m^2)g, e_B f \rangle_N \\ &= \langle (-\Delta + m^2)g, e_B f \rangle_N \\ &= \langle g, e_B f \rangle = 0 \end{aligned}$$

where we have used the definition of $\langle \rangle_N$ in terms of $\langle \rangle$, the fact that $e_A (-\Delta + m^2)g = (-\Delta + m^2)g$, since $(-\Delta + m^2)g$ has support on A_σ , and the fact that $e_B f$ has support on B . This ends the proof of the (pre)Markov property for one-particle systems.

A very important role in the theory is played by subspaces of N associated to hyperplanes in R^4 . To fix ideas, consider the hyperplane $x_4=0$ and the associated subspace N_0 . A tempered distribution in N with support on $x_4=0$ has necessarily the form $(f \otimes \delta_0)(x) \equiv f(x)\delta(x_4)$, with $f \in F$. By using the basic magic formula, for $x \geq 0$ and $M > 0$,

$$\int_{-\infty}^{+\infty} \frac{\exp(ipx)}{p^2 + M^2} dp = \frac{\pi}{M} \exp(-Mx)$$

it is immediate to verify that $\|f \otimes \delta_0\|_N = \|f\|_F$. Therefore, we have an isomorphic and isometric identification of the two Hilbert spaces F and N_0 . Obviously, similar considerations hold for any hyperplane. In particular, we consider the

hyperplanes $x_4=t$ and the associated subspaces N_t . Let us introduce injection operators j_t defined by

$$\begin{aligned} j_t : F &\rightarrow N \\ f &\rightarrow f \otimes \delta_t \end{aligned}$$

where f is a generic element of F , with values $f(x)$, and $(f \otimes \delta_t)(x) = f(x)\delta(x_4 - t)$. It is immediate to verify the following properties for j_t and its adjoint j_t^* : the range of j_t is N_t ; moreover, j_t is an isometry, so that $j_t^* j_t = 1_F, j_t j_t^* = e_t$, where 1_F is the identity on F , and e_t is the projection on N_t . Moreover, $e_t j_t = j_t$ and $j_t^* = j_t^* e_t$.

If we introduce translations $u(t)$ along the x_4 -direction and the reflection r_0 with respect to $x_4=0$, then we also have the covariance property $u(t)j_s = j_{t+s}$, and the reflexivity property $r_0 j_0 = j_0, j_0^* r_0 = j_0^*$. The reflexivity property is very important. It tells us that r_0 leaves N_0 pointwise invariant, and it is an immediate consequence of the fact that $\delta(x_4) = \delta(-x_4)$.

Therefore, if we start from N we can obtain F , by taking the projection j_π with respect to some hyperplane π , in particular $x_4=0$. It is also obvious that we can induce on F a representation of $E(3)$ by taking those elements of $E(4)$ that leave π invariant.

Let us now see how we can define the Hamiltonian on F starting from the properties of N . Since we are considering the simple case of the one-particle system, we could just perform the following construction explicitly by hand, through a simple application of the basic magic formula given earlier. But we prefer to follow a route that emphasizes Markov property and can be immediately generalized to more complicated cases.

Let us introduce the operator $p(t)$ on F defined by the dilation $p(t) = j_0^* j_t = j_0^* u(t) j_0, t \geq 0$. Then we prove the following:

Theorem 2 *The operator $p(t)$ is bounded and self-adjoint. The family $\{p(t)\}$, for $t \geq 0$, is a norm-continuous semigroup.*

Proof Boundedness and continuity are obvious. Self-adjointness is a consequence of reflexivity. In fact,

$$p^*(t) = j_0^* u(-t) j_0 = j_0^* r_0 u(t) r_0 j_0 = j_0^* u(t) j_0 = p(t)$$

The semigroup property is a consequence of the Markov property. In fact, let us introduce N_+, N_0, N_- as subspaces of N made by distributions with support in the regions $x_4 \geq 0, x_4 = 0, x_4 \leq 0$, respectively, and call e_+, e_0, e_- the respective projections. By Markov property, we have $e_0 = e_- e_+$. Now write, for $s, t \geq 0$,

$$p(t)p(s) = j_0^* u(t) j_0 j_0^* u(s) j_0 = j_0^* u(t) e_0 u(s) j_0$$

If e_0 could be cancelled, then the semigroup property would follow from the group property of the translations $u(t)u(s) = u(t+s)$ (a miracle of the dilations!). For this, consider the matrix element

$$\langle f, p(t)p(s)g \rangle_F = \langle u(-t)j_0 f, e_0 u(s)j_0 g \rangle_N$$

recall $e_0 = e_- e_+$, and use $u(s)j_0 g \in N_+$ and $u(-t)j_0 f \in N_-$.

Let us call h the generator of $p(t)$, so that $p(t) = \exp(-th)$, for $t \geq 0$. By definition, h is the Hamiltonian of the physical system. A simple explicit calculation shows that h is just the energy ω introduced earlier. Starting from the representation of the Euclidean group $E(3)$ already given and from the Hamiltonian, we immediately get a representation of the full Poincaré group on F . Therefore, all physical properties of the one-particle system have been reconstructed from its Euclidean image on the Hilbert space N .

As a last remark of this section, let us note that we can consider the real Hilbert spaces N_r and F_r , made of real elements (in configuration space) in N and F . The operators $u(a, t)$, $u(t)$, r_0 , j_π , j_π^* , e_A are all reality preserving, that is, they map real spaces into real spaces.

This completes our discussion about the one-particle system. For more details we refer to Guerra *et al.* (1975) and Simon (1974). We have introduced the Euclidean image, discussed its main properties, and shown how we can derive all properties of the physical system from its Euclidean image. In the next sections, we will show how this kind of construction carries through the second-quantized case and the interacting case.

Second Quantization and Free Fields

We begin this section with a short review about the procedure of second quantization based on probabilistic methods, by following mainly Nelson (1973b); see also Guerra *et al.* (1975) and Simon (1974). Probabilistic methods are particularly useful in the framework of the Euclidean theory.

Let \mathcal{H} be a real Hilbert space with symmetric scalar product $\langle \cdot, \cdot \rangle$. Let $\phi(u)$ be the elements of a family of centered Gaussian random variables indexed by $u \in \mathcal{H}$, uniquely defined by the expectation values $E(\phi(u)) = 0$, $E(\phi(u)\phi(v)) = \langle u, v \rangle$. Since ϕ is Gaussian, we also have

$$E(\exp(\lambda\phi(u))) = \exp(\tfrac{1}{2}\lambda^2\langle u, u \rangle)$$

and

$$E(\phi(u_1)\phi(u_2)\cdots\phi(u_n)) = [u_1 u_2 \cdots u_n]$$

Here $[\dots]$ is the Hafnian of elements $[u_i u_j] = \langle u_i, u_j \rangle$, defined to be zero for odd n , and for even n given by the recursive formula

$$[u_1 u_2 \cdots u_n] = \sum_{i=2}^n [u_1 u_i] [u_1 u_2 \cdots u_n]'$$

where in $[\dots]'$ the terms u_1 and u_i are suppressed. Hafnians, from the Latin name of Copenhagen, the first seat of the theoretical group of CERN, were introduced in quantum field theory by Caianiello (1973), as a useful tool when dealing with Bose statistics.

Let (Q, Σ, μ) be the underlying probability space where ϕ are defined as random variables. Here Q is a compact space, Σ a σ -algebra of subsets of Q , and μ a regular, countable additive probability measure on Σ , normalized to $\mu(Q) = \int_Q d\mu = 1$.

The fields $\phi(u)$ are represented by measurable functions on Q . The probability space is uniquely defined, but for trivial isomorphisms, if we assume that Σ is the smallest σ -algebra with respect to which all fields $\phi(u)$, with $u \in \mathcal{H}$, are measurable. Since $\phi(u)$ are Gaussian, they are represented by $L^p(Q, \Sigma, \mu)$ functions, for any p with $1 \leq p < \infty$, and the expectations will be given by

$$\begin{aligned} E(\phi(u_1)\phi(u_2)\cdots\phi(u_n)) \\ = \int_Q \phi(u_1)\phi(u_2)\cdots\phi(u_n) d\mu \end{aligned}$$

where, by a mild abuse of notation, $\phi(u_i)$ on the right-hand side denote the Q space functions which represent the random variables $\phi(u_i)$. We call the complex Hilbert space $\mathcal{F} = \Gamma(\mathcal{H}) = L^2(Q, \Sigma, \mu)$ the Φ_0 space constructed on \mathcal{H} , and the function $\Omega_0 \equiv 1$ on Q the Φ_0 vacuum.

In order to introduce the concept of second quantization of operators, we must introduce subspaces of \mathcal{F} with a "fixed number of particles." Call $\mathcal{F}_{(0)} = \{\lambda\Omega_0\}$, where λ is any complex number. Define $\mathcal{F}_{(\leq n)}$ as the subspace of \mathcal{F} generated by complex linear combinations of monomials of the type $\phi(u_1)\cdots\phi(u_j)$, with $u_i \in \mathcal{H}$, and $j \leq n$. Then $\mathcal{F}_{(\leq n-1)}$ is a subspace of $\mathcal{F}_{(\leq n)}$. We define $\mathcal{F}_{(n)}$, the n -particle subspace, as the orthogonal complement of $\mathcal{F}_{(\leq n-1)}$ in $\mathcal{F}_{(\leq n)}$, so that

$$\mathcal{F}_{(\leq n)} = \mathcal{F}_{(n)} \oplus \mathcal{F}_{(\leq n-1)}$$

By construction, the $\mathcal{F}_{(n)}$ are orthogonal, and it is not difficult to verify that

$$\mathcal{F} = \bigoplus_{n=0}^{\infty} \mathcal{F}_{(n)}$$

Let us now introduce the Wick normal products by the definition

$$:\phi(u_1)\phi(u_2)\cdots\phi(u_n):=E_{(n)}\phi(u_1)\phi(u_2)\cdots\phi(u_n)$$

where $E_{(n)}$ is the projection on $\mathcal{F}_{(n)}$. It is not difficult to prove the usual Wick theorem (see, e.g., Guerra *et al.* (1975), and its inversion given by Caianiello (1973).

It is interesting to remark that, in the framework of the second quantization performed with probabilistic methods, it is not necessary to introduce creation and destruction operators as in the usual treatment. However, the two procedures are completely equivalent, as shown, for example, in Simon (1974).

Given an operator A from the real Hilbert space \mathcal{H}_1 to the real Hilbert space \mathcal{H}_2 , we define its second-quantized operator $\Gamma(A)$ through the following definitions:

$$\begin{aligned}\Gamma(A)\Omega_{01} &= \Omega_{02} \\ \Gamma(A) : \phi_1(u_1)\phi_1(u_2)\cdots\phi_1(u_n) : \\ &= : \phi_2(Au_1)\phi_2(Au_2)\cdots\phi_2(Au_n) : \end{aligned}$$

where we have introduced the probability spaces \mathcal{Q}_1 and \mathcal{Q}_2 , their vacua Ω_{01} and Ω_{02} , and the random variables ϕ_1 and ϕ_2 , associated to \mathcal{H}_1 and \mathcal{H}_2 , respectively. The following remarkable theorem by Nelson (1973b) gives a full characterization of $\Gamma(A)$, very useful in the applications.

Theorem 3 *Let A be a contraction from the real Hilbert space \mathcal{H}_1 to the real Hilbert space \mathcal{H}_2 . Then $\Gamma(A)$ is an operator from $L^1_{(1)}$ to $L^1_{(2)}$ which is positivity preserving, $\Gamma(A)u \geq 0$ if $u \geq 0$, and such that $E(\Gamma(A)u) = E(u)$. Moreover, $\Gamma(A)$ is a contraction from $L^p_{(1)}$ to $L^p_{(2)}$ for any p , $1 \leq p < \infty$. Finally, $\Gamma(A)$ is also a contraction from $L^p_{(1)}$ to $L^q_{(2)}$, with $q \geq p$, if $\|A\|^2 \leq (p-1)/(q-1)$.*

We have indicated with $L^p_{(1)}, L^p_{(2)}$ the L^p spaces associated to \mathcal{H}_1 and \mathcal{H}_2 , respectively. This is the celebrated best hypercontractive estimate given by Nelson. For the proof, we refer to the original paper of Nelson (1973b); see also Simon (1974).

This completes our short review on the theory of second quantization based on probabilistic methods.

The usual time-zero quantum field $\bar{\phi}(u), u \in F_r$, in the Φ_0K representation, can be obtained through second quantization starting from F_r . We call $(\bar{Q}, \bar{\Sigma}, \bar{\mu})$ the underlying probability space, and $\mathcal{F} = \Gamma(F_r) = L^2(\bar{Q}, \bar{\Sigma}, \bar{\mu})$ the Hilbert Φ_0K space of the free physical particles.

Now we introduce the free Markov field $\phi(f), f \in N_r$, by taking N_r as the starting point. We call (Q, Σ, μ) the associated probability space. We

introduce the Hilbert space $\mathcal{N} = \Gamma(N_r) = L^2(Q, \Sigma, \mu)$, and the operators $U(a, R) = \Gamma(u(a, R))$, $R_0 = \Gamma(r_0)$, $U(t) = \Gamma(u(t))$, $E_A = \Gamma(e_A)$, and so on, for which the previous Nelson theorem holds (take $\mathcal{H}_1 = \mathcal{H}_2 = N_r$).

Since in general $\Gamma(AB) = \Gamma(A)\Gamma(B)$, we have immediately the following expression of the Markov property $E_\sigma = E_A E_B$, where the closed regions A, B, σ of the Euclidean space have the same properties as explained earlier in the proof of the (pre)Markov property for one-particle systems.

It is obvious that E_A can also be understood as conditional expectation with respect to the sub- σ -algebra Σ_A generated by the field $\phi(f)$ with $f \in N_r$ and the support of f on A .

The relation, previously pointed out, between N_t subspaces and F are also valid for their real parts N_{rt} and F_r . Therefore, they carry out through the second quantization procedure. We introduce $J_t = \Gamma(j_t)$ and $J_t^* = \Gamma(j_t^*)$; then the following properties hold. J_t is an isometric injection of $L^p(\bar{Q}, \bar{\Sigma}, \bar{\mu})$ into $L^p(Q, \Sigma, \mu)$; the range of J_t as an operator $L^2 \rightarrow L^2$ is obviously $\mathcal{N}_t = \Gamma(N_{rt})$; moreover, $J_t J_t^* = E_t$. The free Hamiltonian H_0 is given for $t \geq 0$ by

$$J_0^* J_t = \exp(-tH_0) = \Gamma(\exp(-t\omega))$$

Moreover, we have the covariance property $U(t)J_0 = J_t$, and the reflexivity $R_0 J_0 = J_0, J_0^* R_0 = J_0^*$.

These relations allow a very simple expression for the matrix elements of the Hamiltonian semigroup in terms of Markov quantities. In fact, for $u, v \in \mathcal{F}$ we have

$$\langle u, \exp(-tH_0)v \rangle = \int_{\bar{Q}} (J_t u)^* J_0 v \, d\mu$$

In the next section, we will generalize this representation to the interacting case.

Finally, let us derive the hypercontractive property of the free Hamiltonian semigroup.

Since $\|\exp(-t\omega)\| \leq \exp(-tm)$, where m is the mass of the particle, we have immediately, by a simple application of Nelson theorem,

$$\|\exp(-tH_0)\|_{p,q} \leq 1$$

provided $q-1 \leq (p-1)\exp(2tm)$, where $\|\dots\|_{p,q}$ denotes the norm of an operator from L^p to L^q spaces.

Interacting Fields

The discussion of the previous sections was limited to free fields both in Minkowski and Euclidean spaces. Now we must introduce interaction in order to get nontrivial theories.

First, as a general motivation, we will proceed quite formally and then we will resort to precise statements.

Let us recall that in standard quantum field theory, for scalar self-coupled fields, the time-ordered products of quantum fields in Minkowski spacetime can be expressed formally through the formula

$$\frac{\langle T(\phi(x_1) \cdots \phi(x_n) \exp(i \int \mathcal{L} dx)) \rangle}{\langle T \exp(i \int \mathcal{L} dx) \rangle}$$

where T denotes time ordering, ϕ are free fields in Minkowski spacetime, \mathcal{L} is the interaction Lagrangian, and $\langle \dots \rangle$ are vacuum averages. As is well known, this expression can be put, for example, at the basis of perturbative expansions, giving rise to terms expressed through Feynman graphs. The appropriately chosen normalization provides automatic cancelation of the vacuum to vacuum graphs.

Now we can introduce a formal analytic continuation to the Schwinger points, as previously done for the one-particle system, and obtain the following expression for the analytic continuation of the field time-ordered products, now called Schwinger functions,

$$S(x_1, \dots, x_n) = \frac{\langle \phi(x_1) \cdots \phi(x_n) \exp U \rangle}{\langle \exp U \rangle}$$

Here x_1, \dots, x_n denote points in Euclidean space, ϕ are the Euclidean fields introduced earlier. The chronological time ordering disappears, because the fields ϕ are commutative, and there is no distinguished "time" direction in Euclidean space. Here the symbol $\langle \dots \rangle$ denotes the expectation values represented by $\int \dots d\mu$, as explained earlier, and U is the Euclidean "action" of the system formally given by the integral on Euclidean space

$$U = - \int P(\phi(x)) dx$$

if the field self-interaction is produced by the polynomial P .

Therefore, these formal considerations suggest that the passage from the free Euclidean theory to the fully interacting one is obtained through a change of the free probability measure $d\mu$ to the interacting measure

$$\exp U d\mu / \int_Q \exp U d\mu$$

The analogy with classical statistical mechanics is evident. The expression $\exp U$ acts as Boltzmannfaktor, and $Z = \int_Q \exp U d\mu$ is the partition function.

Our task will be to make these statements precise from a mathematical point of view. We will be

obliged to introduce cutoffs, and then be involved in their careful removal.

For the sake of convenience, we make the substantial simplification of considering only two-dimensional theories (one space, one time dimension in the Minkowski region) for which the well-known ultraviolet problem of quantum field theory gives no trouble. There is no difficulty in translating the contents of the previous sections to the two-dimensional case.

Let P be a real polynomial, bounded below and normalized to $P(0)=0$. We introduce approximations h to the Dirac δ function at the origin of the two-dimensional Euclidean space R^2 , with $h \in N_r$. Let h_x be the translate of h by x , with $x \in R^2$. The introduction of h , equivalent to some ultraviolet cutoff, is necessary, because local fields, of the formal type $\phi(x)$, have no rigorous meaning, and some smearing is necessary.

For some compact region Λ in R^2 , acting as space cutoff (infrared cutoff), introduce the Q space function

$$U_\Lambda^{(h)} = - \int_\Lambda :P(\phi(h_x)): dx$$

where dx is the Lebesgue measure in R^2 . It is immediate to verify that $U_\Lambda^{(h)}$ is well defined, bounded below and belongs to $L^p(Q, \Sigma, \mu)$, for any p , $1 \leq p < \infty$. This is the infrared and ultraviolet cutoff action. Notice the presence of the Wick normal products in its definition. They provide a kind of automatic introduction of counterterms, in the framework of renormalization theory.

The following theorem allows us to remove the ultraviolet cutoff.

Theorem 4 *Let $h \rightarrow \delta$, in the sense that the Fourier transforms \tilde{h} are uniformly bounded and converge pointwise in momentum space to the Fourier transform of the δ -function given by $(2\pi)^{-2}$. Then $U_\Lambda^{(h)}$ is L^p -convergent for any p , $1 \leq p < \infty$, as $h \rightarrow \delta$. Call U_Λ the L^p -limit, then $U_\Lambda, \exp U_\Lambda \in L^p(Q, \Sigma_\Lambda, \mu)$, for $1 \leq p < \infty$.*

The proof uses standard methods of probability theory, and originates from pioneering work of Nelson in (1966). It can be found for example in Guerra *et al.* (1975), and Simon (1974).

Since U_Λ is defined with normal products, and the interaction polynomial P is normalized to $P(0)=0$, an elementary application of Jensen inequality gives

$$\int_Q \exp U_\Lambda d\mu \geq \exp \cdot \int_Q U_\Lambda d\mu = 1$$

Therefore, we can rigorously define the new space cutoff measure in Q space:

$$d\mu_\Lambda = \exp U_\Lambda d\mu / \int_Q \exp U_\Lambda d\mu$$

The space-cutoff interacting Euclidean theory is defined by the same fields on Q space, but with a change in the measure and, therefore, in the expectation values. The correlations for the interacting fields $\bar{\phi}$ are the cutoff Schwinger functions

$$\begin{aligned} S_\Lambda(x_1, \dots, x_n) &= \langle \bar{\phi}(x_1) \cdots \bar{\phi}(x_n) \rangle \\ &= Z_\Lambda^{-1} \langle \phi(x_1) \cdots \phi(x_n) \exp U_\Lambda \rangle \end{aligned}$$

where the partition function is

$$Z_\Lambda = \langle \exp U_\Lambda \rangle$$

We see that the analogy with statistical mechanics is complete here. Of course, the introduction of the space cutoff Λ destroys translation invariance. The full Euclidean covariant theory must be recovered by taking the infinite-volume limit $\Lambda \rightarrow R^2$ on field correlations. For the removal of the space cutoff, all methods of statistical mechanics are available. In particular, correlation inequalities of ferromagnetic type can be easily exploited, as shown, for example, in Guerra *et al.* (1975) and Simon (1974).

We would like to conclude this section by giving the connection between the space-cutoff Euclidean theory and the space-cutoff Hamiltonian theory in the physical Φ_0 space.

For $\ell \geq 0, t \geq 0$, consider the rectangle in R^2 ,

$$\Lambda(\ell, t) = \left\{ (x_1, x_2) : -\frac{\ell}{2} \leq x_1 \leq \frac{\ell}{2}, 0 \leq x_2 \leq t \right\}$$

and define the operator in the physical Φ_0 space

$$P_\ell(t) = J_0^* \exp U_\Lambda(\ell, t) J_t$$

where J_0 and J_t are injections relative to the lines $x_2 = 0$ and $x_2 = t$, respectively. Then the following theorem, largely due to Nelson, holds.

Theorem 5 *The operator $P_\ell(t)$ is bounded and self-adjoint. The family $\{P_\ell(t)\}$, for ℓ fixed and $t \geq 0$, is a strongly continuous semigroup. Let H_ℓ be its lower bounded self-adjoint generator, so that $P_\ell(t) = \exp(-tH_\ell)$. On the physical Φ_0 space, there is a core \mathcal{D} for H_ℓ such that on \mathcal{D} the equality $H_\ell = H_0 + V_\ell$ holds, where H_0 is the free Hamiltonian introduced earlier and V_ℓ is the volume-cutoff interaction given by*

$$V_\ell = \lim \int_{-\ell/2}^{\ell/2} : P(\bar{\phi}(h_{x_1})) : dx_1$$

where h_{x_1} are the translates of approximations to the δ -function at the origin on the x_1 -space, and the limit is taken in L^p , in analogy to what has been explained for the two-dimensional case in the definition of U_Λ .

While we refer to Guerra *et al.* (1975) and Simon (1974) for a full proof, we mention here that boundedness is related to hypercontractivity of the free Hamiltonian, self-adjointness is a consequence of reflexivity, and the semigroup property follows from Markov property. This theorem is remarkable, because it expresses the cutoff interacting Hamiltonian semigroup in an explicit form in the Euclidean theory through probabilistic expectations. In fact, we have

$$\langle u, \exp(-tH_\ell)v \rangle = \int_Q (J_t u)^* J_0 v \exp U_\Lambda(\ell, t) d\mu$$

We could call this expression as the Feynman–Kac–Nelson formula, in fact it is nothing but a path integral expressed in stochastic terms, and adapted to the Hamiltonian semigroup.

By comparison with the analogous formula given for the free Hamiltonian semigroup, we see that the introduction of the interaction inserts the *Boltzmannfaktor* under the integral.

As an immediate consequence of the Feynman–Kac–Nelson formula, together with Euclidean covariance, we have the following astonishing Nelson symmetry:

$$\langle \Omega_0, \exp(-tH_\ell)\Omega_0 \rangle = \langle \Omega_0, \exp(-\ell H_t)\Omega_0 \rangle$$

which was at the basis of Guerra (1972) and Guerra *et al.* (1972), and played some role in showing the effectiveness of Euclidean methods in constructive quantum field theory.

It is easy to establish, through simple probabilistic reasoning, that H_ℓ has a unique ground state Ω_ℓ of lowest energy E_ℓ . For a convenient choice of normalization and phase factor, one has $\|\Omega_\ell\|_2 = 1$, and $\Omega_\ell > 0$ almost everywhere on Q space (for bosonic systems, ground states have no nodes in configuration space!). Moreover, $\Omega_\ell \in L^p$, for any $1 \leq p < \infty$. If $\ell > 0$ and the interaction is not trivial, then $\Omega_\ell \neq \Omega_0, E_\ell < 0$, and $\|\Omega_\ell\|_1 < 1$. Obviously, $\|\exp(-tH_\ell)\|_{2,2} = \exp(-tE_\ell)$.

The general structure of Euclidean field theory, as explained in this section, has been at the basis of all applications in constructive quantum field theory. These applications include the proof of the existence of the infinite-volume limit, with the establishment of all Wightman axioms, for two- and three-dimensional theories. Moreover, the existence of phase transitions and symmetry breaking has been firmly established.

Extensions have also been given to theories involving Fermions, and to gauge field theory. Due to the scope of this review, limited to a description of the general structure of Euclidean field theory, we cannot give a detailed treatment of these applications. Therefore, we refer to recent general reviews on constructive quantum field theory for a complete description of all results (see, e.g., Jaffe (2000)). For recent applications of Euclidean field theory to quantum fields on curved spacetime manifolds we refer, for example, to Schlingemann (1999).

The Physical Interpretation of Euclidean Field Theory

Euclidean field theory has been considered by most researchers as a very useful tool for the study of quantum field theory. In particular, it is quite easy, for example, to obtain the fully interacting Schwinger functions in the infinite-volume limit in two-dimensional spacetime. At this point, there arises the problem of connecting these Schwinger functions with observable physical quantities in Minkowski spacetime. A very deep result of Osterwalder and Schrader (1973) gives a very natural interpretation of the resulting limiting theory. In fact, the Euclidean theory, as has been shown earlier, arises from an analytic continuation from the physical Minkowski spacetime to the Schwinger points, through a kind of analytic continuation in time (also called Wick rotation, because Wick exploited this trick in the study of the Bethe-Salpeter equation). Therefore, having obtained the Schwinger functions for the full covariant theory, after all cutoff removal, it is very natural to try to reproduce the inverse analytic continuation in order to recover the Wightman functions in Minkowski spacetime. Therefore, Osterwalder and Schrader have been able to identify a set of conditions, quite easy to verify, which allow us to recover Wightman functions from Schwinger functions. A key role in this reconstruction theorem is played by the so-called reflection positivity for Schwinger functions, a property quite easy to verify. In this way, a fully satisfactory solution for the physical interpretation of Euclidean field theory is achieved.

From a historical point of view, an alternate route is possible. In fact, at the beginning of the exploitation of Euclidean methods in constructive quantum field theory, Nelson was able to isolate a set of axioms for the Euclidean *fields* (Nelson 1973a), allowing the reconstruction of the physical theory. Of course, Nelson axioms are more difficult to

verify, since they also involve properties of the Euclidean fields and not only of the Schwinger functions. However, it is still very interesting to investigate whether the Euclidean fields play only an auxiliary role in the construction of the physical content of relativistic theories, or if they have a more fundamental meaning.

From a physical point of view, the following considerations could also lead to further developments along this line. By its very structure, the Euclidean theory contains the fixed-time quantum correlations in the vacuum. In elementary quantum mechanics, it is possible to derive all physical content of the theory from the simple knowledge of the ground state wave function, including scattering data. Therefore, at least in principle, it should be possible to derive all physical content of the theory directly from the Euclidean theory, without any analytic continuation.

We conclude this short section on the physical interpretation of the Euclidean theory with a mention of a quite surprising result (Guerra and Ruggiero 1973) obtained by submitting classical field theory to the procedure of stochastic quantization in the sense of Nelson (1985). The procedure of stochastic quantization associates a stochastic process to each quantum state. In this case, in a fixed reference frame, the procedure of stochastic quantization, applied to interacting fields, produces, for the ground state, a process in the physical spacetime that has the same correlations as Euclidean field theory. This opens the way to a possible interpretation of Euclidean field theory directly in Minkowski spacetime. However, a consistent development along this line requires a new formulation of representations of the Poincaré group in the form of measure-preserving transformations in the probability space where the Euclidean fields are defined. This difficult task has not been accomplished as yet.

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See also: Axiomatic Quantum Field Theory; Constructive Quantum Field Theory; Feynman Path Integrals; Functional Integration in Quantum Physics; High T_c Superconductor Theory; Malliavin Calculus; Quantum Chromodynamics; Quantum Field Theory: A Brief Introduction; Quantum Fields with Indefinite Metric; Non-Trivial Models; Relativistic Wave Equations including Higher Spin Fields; Renormalization: General Theory; Two-dimensional Models.

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Evolution Equations: Linear and Nonlinear

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Introduction

In this article we present the semigroup approach to linear and nonlinear evolution equations in general Banach spaces. In the first part we introduce the general frame and we explain the cornerstones of the widely developed theory of linear evolution equations. Besides the classical approach to linear evolution equations based on C_0 -semigroups, we also give a brief introduction to the more recent theory of maximal regularity. The entire linear theory is not only important on its own (which we prove by discussing applications to the heat equation, Schrödinger equation, wave equation, and Maxwell equations) but it is also the indispensable basis for the theory of nonlinear evolution equation, which we present in the second part.

Linear Evolution Equations

Let E_0 be a Banach space, $T > 0$, and assume that $\mathcal{A} := \{A(t); t \in [0, T]\}$ is a family of closed linear operators in E_0 . By this we mean that, given $t \in [0, T]$, there is a linear subspace $D(A(t))$ of E_0 and

linear mapping $A(t) : D(A(t)) \subset E_0 \rightarrow E_0$ such that the graph $\{(x, A(t)x); x \in D(A(t))\}$ of $A(t)$ is a closed subspace of $E_0 \times E_0$. Given a mapping $f : [0, T] \rightarrow E_0$ and a vector $u_0 \in E_0$, we study the following initial-value problem for (\mathcal{A}, f, u_0) : find a function $u \in C^1([0, T], E_0)$ such that $u(t) \in D(A(t))$ for $t \in (0, T]$ and

$$u'(t) = A(t)u(t) + f(t), \quad t \in (0, T], \quad u(0) = u_0 \quad [1]$$

Sometimes we call [1] also the Cauchy problem of the linear evolution equation $u'(t) = A(t)u(t) + f(t)$. In the following, we will specify different conditions on (\mathcal{A}, f, u_0) which guarantee the well-posedness of [1], and we shall discuss several examples of equations of type [1] which are relevant in mathematical physics.

Autonomous Homogeneous Equations

As in the case of ordinary differential equations in finite-dimensional spaces, it is convenient to consider first the autonomous version of [1], that is, we assume that \mathcal{A} is trivial in the sense that $T = \infty$ and that $A(0) = A(t)$ for all $t \geq 0$. In order to simplify our notation, we set $A := A(0)$. We consider first the homogeneous problem

$$u'(t) = Au(t), \quad t \in (0, \infty), \quad u(0) = u_0 \quad [2]$$

where $u_0 \in E_0$ is given. The question of the well-posedness of [2] is closely tied to the notion of a C_0 -semigroup in E_0 . Let $\mathcal{L}(E_0)$ denote the Banach space of all bounded linear operators on E_0 , endowed with the usual operator norm. A one-parameter family $\mathcal{T} = \{T(t) \in \mathcal{L}(E_0); t \geq 0\}$ is called “ C_0 -semigroup” in $\mathcal{L}(E_0)$ iff

1. $T(0) = \text{id}_{E_0}$ (normalization),
2. $T(s+t) = T(s)T(t)$ for all $s, t \geq 0$ (semigroup property), and
3. $\lim_{t \rightarrow 0} T(t)x = x$ for all $x \in E_0$ (strong continuity at 0).

Given a C_0 -semigroup \mathcal{T} , we define its (infinitesimal) generator B by setting

$$\text{dom}(B) := \left\{ x \in E_0; \lim_{t \rightarrow 0} \frac{T(t)x - x}{t} \text{ exists in } E_0 \right\}$$

and by defining

$$Bx := \lim_{t \rightarrow 0} \frac{T(t)x - x}{t} \quad \text{for } x \in \text{dom}(B)$$

This clearly defines a linear operator in E_0 and it is well known that B is closed and densely defined. Moreover, we have

Theorem 1 Assume that $A: D(A) \subset E_0 \rightarrow E_0$ is the generator of a C_0 -semigroup $\{T(t); t \geq 0\}$. Then, given $u_0 \in D(A)$, problem [2] possesses a unique solution u in $C^1([0, \infty), E_0)$, which is given by $u(t) = T(t)u_0$.

Under suitable additional assumptions it can be shown that the converse of Theorem 1 also holds true. However, we shall not go into these details but we prefer to present the following characterization of generators of C_0 -semigroups:

Theorem 2 (Hille–Yosida). The operator $A: D(A) \subset E_0 \rightarrow E_0$ generates a C_0 -semigroup iff it is closed, densely defined, and there exists $\omega, M \in \mathbb{R}$ such that the resolvent set $\rho(A)$ of A contains the ray (ω, ∞) and such that $\|(\lambda - \omega)^n(\lambda - A)^{-n}\| \leq M$ for all $\lambda > \omega$ and all $n \in \mathbb{N}$.

In applications, it is in general rather difficult to derive a uniform estimate of powers of the resolvent of an unbounded operator. Luckily, generators of C_0 -semigroups of contractions (i.e., $\|T(t)\|_{\mathcal{L}(E_0)} \leq 1$ for all $t \geq 0$) can be characterized in a rather useful way. To formulate this result we call an operator $B: D(B) \subset E_0 \rightarrow E_0$ “dissipative” iff for any $x \in D(B)$ there is an $x' \in E'_0$ with $\langle x', x \rangle = \|x\|_{E_0}^2 = \|x'\|_{E'_0}^2$ such that $\text{Re} \langle x', Bx \rangle \leq 0$. Here $\langle \cdot, \cdot \rangle$ denotes the duality pairing between E'_0 and E_0 . The operator B is called “ m -dissipative” if it is dissipative and $\text{im}(\lambda_0 - A) = E_0$ for some $\lambda_0 > 0$.

Theorem 3 (Lumer–Phillips). Let $A: D(A) \subset E_0 \rightarrow E_0$ be a closed and densely defined operator. Then A generates a C_0 -semigroup of contractions in $\mathcal{L}(E_0)$ iff A is m -dissipative.

Before we shall discuss examples of C_0 -semigroups and their infinitesimal generators, let us introduce the following definition: given $\alpha \in (0, \pi]$, let $\Sigma_\alpha := \{z \in \mathbb{C}; |\arg(z)| < \alpha\}$ denote the sector in \mathbb{C} of angle 2α . A family of operators $\mathcal{T} = \{T(z) \in \mathcal{L}(E_0); z \in \Sigma_\alpha\}$ is called a “holomorphic C_0 -semigroup” in $\mathcal{L}(E_0)$ iff

1. $[z \mapsto T(z)]: \Sigma_\alpha \rightarrow \mathcal{L}(E_0)$ is holomorphic,
2. $T(0) = \text{id}_{E_0}$ and $\lim_{z \rightarrow 0} T(z)x = x$ for all $x \in E_0$, and
3. $T(w+z) = T(w)T(z)$ for all $w, z \in \Sigma_\alpha$.

Generators of holomorphic C_0 -semigroups can be characterized in the following way:

Theorem 4 A densely defined closed linear operator $A: D(A) \subset E_0 \rightarrow E_0$ generates a holomorphic C_0 -semigroup iff there exist $M > 0$ and $\omega_0 \geq 0$ such that $\lambda \in \rho(A)$ and $\|\lambda(\lambda - A)^{-1}\| \leq M$ for all $\lambda \in \mathbb{C}$ with $\text{Re } \lambda > \omega_0$.

Examples 5

(i) *Self-adjoint generators.* Let E_0 be a Hilbert space and assume that A is self-adjoint and that there exists an $\alpha_0 \in \mathbb{R}$ such that $A \leq \alpha_0$. Then A generates a holomorphic C_0 -semigroup $\{T(t); t \geq 0\}$. If $\{E_A(\lambda); \lambda \in \mathbb{R}\}$ denotes the spectral resolution of A , then $T(t) = \int_{\mathbb{R}} \exp(t\lambda) dE_A(\lambda)$ for $t \geq 0$.

(ii) *Dissipative operators in Hilbert spaces.* Assume again that E_0 is a Hilbert space. Then, by Riesz’ representation formula, an operator A is dissipative iff $\text{Re}(u|Au) \leq 0$ for all $u \in D(A)$.

(iii) *The heat semigroup.* Let M be either a smooth compact closed Riemannian manifold or \mathbb{R}^m with the Euclidean metric and write Δ for the Laplace–Beltrami operator on M . Then it is known that $\Delta \in \mathcal{L}(\mathcal{D}'(M))$, where $\mathcal{D}'(M)$ is the space of all distributions on M . Given $1 \leq p < \infty$, let

$$D(\Delta_p) := \{u \in L_p(M); \Delta u \in L_p(M)\}$$

and set $\Delta_p u = \Delta u$ for $u \in D(\Delta_p)$. Then Δ_p generates a holomorphic C_0 -semigroup on $L_p(M)$, the so-called “diffusion” or “heat semigroup” on M . If $1 < p < \infty$, then it can be shown that $D(\Delta_p) = W_p^2(M)$, where $W_p^k(M)$ denotes the Sobolev space of order $k \in \mathbb{N}$, built over $L_p(M)$.

If $M = \mathbb{R}^m$ then the operators $T(t)$ of the semigroup generated by $\Delta_{\mathbb{R}^m}$ are given by

$$T(t)u(x) = \frac{1}{(4\pi t)^{m/2}} \int_{\mathbb{R}^m} \exp\left(\frac{-|x-y|^2}{4t}\right) u(y) dy$$

for all $t > 0$ and almost all $x \in \mathbb{R}^m$.

Observe that the case $L_\infty(M)$ is excluded here. In fact, it is known that if a linear operator A generates a C_0 -semigroup on $L_\infty(M)$, then A must be bounded. However, it can be shown that suitable realizations of the Laplace–Beltrami operator on spaces of continuous and Hölder continuous functions generate holomorphic semigroups. For more details on that topic the reader is referred to the “Further reading” section.

(iv) *Stone’s theorem and the Schrödinger equation.* Let E_0 be a Hilbert space and assume that A is self-adjoint. Then Theorem 3 and Remark (ii) imply that iA generates a C_0 -group $\{U(t); t \in \mathbb{R}\}$ of unitary operators. In fact, Stone’s theorem ensures that every generator of a C_0 -group of unitary operators is of the form iA with a self-adjoint operator A . As an example of particular interest, let us consider the Schrödinger equation

$$\frac{1}{i} \frac{\partial u}{\partial t} = \Delta u - Vu \quad [3]$$

with a bounded potential $V: \mathbb{R}^m \rightarrow \mathbb{R}$. Letting $D(A) := H^2(\mathbb{R}^m)$ and $Au := \Delta u - Vu$, it follows that A is self-adjoint in $L_2(\mathbb{R}^m)$. Hence, the evolution of [3] is governed by the group of unitary operators generated by iA . Of course, the assumption that V be bounded is rather restrictive. In fact, there are numerous contributions which show that this assumption can be weakened considerably. Again reader is referred to the “Further reading” section for more details in this direction.

(v) *The wave equation.* Let us consider the following initial-value problem

$$\begin{aligned} \square u(t, x) &= 0, \quad x \in \mathbb{R}^m, \quad t > 0 \\ u(0, x) &= \varphi_1(x), \quad \partial u / \partial t(0, x) \\ &= \varphi_2(x), \quad x \in \mathbb{R}^m \end{aligned} \quad [4]$$

for the d’Alembert operator $\square = \partial^2 u / \partial t^2 - \Delta_{\mathbb{R}^m}$ in $m + 1$ dimensions. In order to associate with [4] a semigroup, let us formally re-express [4] as the following first-order system:

$$\frac{dU}{dt} = AU, \quad t > 0, \quad U(0) = \Phi$$

where

$$U = (u, u'), \quad A = \begin{pmatrix} 0 & \text{id} \\ \Delta & 0 \end{pmatrix}, \quad \Phi = (\varphi_1, \varphi_2)$$

Letting now $E_0 := H^1(\mathbb{R}^m) \times L_2(\mathbb{R}^m)$ and $D(A) := H^2(\mathbb{R}^m) \times H^1(\mathbb{R}^m)$, it can be shown that A generates a C_0 -group of linear operators in $\mathcal{L}(E_0)$. Hence, given any initial datum $(\varphi_1, \varphi_2) \in H^2(\mathbb{R}^m) \times H^1(\mathbb{R}^m)$, there exists a unique solution $u \in C^1([0, \infty), L_2(\mathbb{R}^m))$ to the initial-value problem [4]. It

can be shown that this solution possesses the following additional regularity:

$$u \in C^2([0, \infty), L_2(\mathbb{R}^m)) \cap C([0, \infty), H^2(\mathbb{R}^m))$$

Hence, eqns [4] are satisfied for all $t \in [0, \infty)$ and for almost all $x \in \mathbb{R}^m$.

(vi) *Maxwell equations.* Let E and H denote the electric and magnetic field vector, respectively, ε and μ the electrical permittivity and magnetic permeability, respectively, and consider the initial-value problem for Maxwell equations in vacuum and without charges and currents: given sufficiently smooth vector fields (E_0, H_0) find a pair (E, H) such that

$$\begin{aligned} \varepsilon \frac{\partial E}{\partial t} - \text{rot } H &= 0 \quad \text{in } (0, \infty) \times \mathbb{R}^3 \\ \mu \frac{\partial H}{\partial t} + \text{rot } E &= 0 \quad \text{in } (0, \infty) \times \mathbb{R}^3 \\ E(0, \cdot) &= E_0, \quad H(0, \cdot) = H_0 \quad \text{in } \mathbb{R}^3 \end{aligned} \quad [5]$$

We assume that ε and μ belong to $L_\infty(\mathbb{R}^3, \mathcal{L}_{\text{sym}}(\mathbb{R}^3))$ and are uniformly positive definite, that is, we assume that there are $\varepsilon_0 > 0$ and $\mu_0 > 0$ such that

$$(\varepsilon(x)y|y) \geq \varepsilon_0|y|^2, \quad (\mu(x)y|y) \geq \mu_0|y|^2$$

for all $x, y \in \mathbb{R}^3$. Based on these assumptions we endow the space $L_2(\mathbb{R}^3) \times L_2(\mathbb{R}^3)$ with the inner product

$$((u_1, u_2)|(v_1, v_2)) := (\varepsilon u_1|v_1)_{L_2} + (\mu u_2|v_2)_{L_2}$$

for $(u_1, u_2), (v_1, v_2) \in L_2(\mathbb{R}^3) \times L_2(\mathbb{R}^3)$, and call this Hilbert space E_0 . We further set

$$E_1 := \{(u_1, u_2) \in E_0; (\text{rot } u_1, \text{rot } u_2) \in E_0\}$$

Finally, given $u = (u_1, u_2) \in E_1$, let

$$Au := (\varepsilon^{-1} \text{rot } u_2, -\mu^{-1} \text{rot } u_1)$$

It can be shown that iA is self-adjoint in E_0 . Hence, Stone’s theorem ensures that A generates a C_0 -group of unitary operators in $\mathcal{L}(E_0)$. Therefore, given $(E_0, H_0) \in E_1$, there exists a unique solution $(E(\cdot), H(\cdot))$ of [5]. For this solution, the energy functional

$$E(t) = \frac{1}{2} \int_{\mathbb{R}^3} [(\varepsilon E(t)|E(t))_{\mathbb{R}^3} + (\mu H(t)|H(t))_{\mathbb{R}^3}] dx$$

is constant on $[0, \infty)$.

Autonomous Inhomogeneous Equations

Next, we study problem [1] in the case $A(t) = A$ for all $t \in [0, T)$. Throughout this section we assume that the following minimal hypotheses

1. A generates a C_0 -semigroup in $\mathcal{L}(E_0)$,
2. $f \in L_1((0, T), E_0)$, and
3. $u_0 \in E_0$

are satisfied. Later on we shall discuss several more restrictive assumptions on (A, f, u_0) . A function $u: [0, T] \rightarrow E_0$ is called a “(classical) solution” of

$$u'(t) = Au(t) + f(t), \quad t \in (0, T], \quad u(0) = u_0 \quad [6]$$

iff $u \in C([0, T], E_0) \cap C^1((0, T], E_0)$, $u(t) \in D(A)$ for all $t \in (0, T]$, and u satisfies [6] pointwise on $[0, T]$. It can be shown that [6] has at most one solution. If it has a solution, this solution is represented by the following variation-of-constant-formula:

$$u(t) = T(t)u_0 + \int_0^t T(t-s)f(s) ds, \quad t \in [0, T] \quad [7]$$

where $\{T(t); t \geq 0\}$ denotes the semigroup generated by A . Observe that the function $u: [0, T] \rightarrow E_0$, defined by [7], is continuous, but in general not differentiable on $(0, T]$. For this reason one calls [7] the “mild solution” of [6].

It is not difficult to see that if $u_0 \in D(A)$ and $f \in C^1([0, T], E_0)$, then the mild solution is a classical solution, that is, [6] is uniquely solvable in the classical sense. In application to nonlinear problems, the assumption $f \in C^1([0, T], E_0)$ is often too restrictive. Fortunately, in the case of generators of holomorphic semigroups, this assumption on f can be weakened in two different directions. Let $\|x\|_A := \|x\|_{E_0} + \|Ax\|_{E_0}$ denote the graph norm on $D(A)$. Then the closedness of A implies that $(D(A); \|\cdot\|_A)$ is a Banach space. In the following, we call this Banach space E_1 . Moreover, given $\alpha \in (0, 1)$, we write $E_\alpha = (E_0, E_1)_\alpha$ for the complex interpolation space between E_0 and E_1 . Then we have the following result.

Theorem 6 *Let A generate a holomorphic C_0 -semigroup in $\mathcal{L}(E_0)$ and assume that there is a constant $\alpha \in (0, 1)$ such that*

$$f \in C^\alpha([0, T], E_0) + C([0, T], E_\alpha)$$

Then, given $u_0 \in E_0$, the Cauchy problem [6] possesses a unique classical solution. It is given by

$$u(t) = T(t)u_0 + \int_0^t T(t-s)f(s) ds, \quad t \in [0, T]$$

where $\{T(t); t \geq 0\}$ stands for the semigroup generated by A .

In the following, we discuss an alternative approach to the Cauchy problem [6], which is based on the so-called theory of maximal regularity. There are several different types of results on maximal regularity, which we cannot discuss in full detail here. We decided to give a brief introduction to the theory of the so-called “maximal L_p -regularity.” For further results on maximal regularity, we

again draw the reader’s attention to the “Further reading” section.

The Banach space E_0 is called an unconditionality of martingale “differences” (UMD) space if the Hilbert transform is bounded on $L_q(\mathbb{R}, E_0)$ for some $q \in (1, \infty)$. It is known that Hilbert spaces, the Lebesgue spaces $L_p(X, d\mu)$ with $1 < p < \infty$ and with a σ -finite measure space (X, μ) , and closed subspaces of UMD spaces are UMD spaces. Furthermore, UMD spaces are without exception reflexive. Thus, the spaces $L_1(X, d\mu)$, $L_\infty(X, d\mu)$, and spaces of continuous or Hölder continuous functions are not UMD spaces.

Next, assume that $-A$ generates a holomorphic C_0 -semigroup in $\mathcal{L}(E_0)$ and that $[0, \infty) \subset \rho(-A)$. Then, it is known that, given $z \in \mathbb{C}$, the fractional power A^z of A is a densely defined closed operator in E_0 . We say that A has bounded imaginary powers (BIP) of angle $\theta \geq 0$ if there exist positive constants M and ε such that

$$A^{it} \in \mathcal{L}(E_0) \quad \text{and} \quad \|A^{it}\|_{\mathcal{L}(E_0)} \leq M \exp(\theta|t|) \quad [8]$$

$$t \in (-\varepsilon, \varepsilon)$$

In order to have a neat notation, we write $A \in \text{BIP}(\theta)$ if [8] holds true.

Remarks 7 In the following, we assume that $-A$ generates a holomorphic C_0 -semigroup in $\mathcal{L}(E_0)$ and that $[0, \infty) \subset \rho(-A)$.

- (i) If $\text{Re } z < 0$, then A^z is bounded on E_0 .
- (ii) There are several representation formulas for the fractional powers of A . Among them we picked the following: if $\text{Re } z \in (-1, 1)$ and $x \in D(A)$, then

$$A^z x = \frac{\sin(\pi z)}{\pi z} \int_0^\infty s^z (s + A)^{-2} A x \, ds$$

- (iii) Assume that E_0 is a Hilbert space, that A is self-adjoint, and that there is a positive constant α such that $A \geq \alpha$. Further, let $\{E_A(\lambda) \in \mathbb{R}\}$ be the spectral resolution of A ; then

$$A^z := \int_0^\infty \lambda^z dE_A(\lambda), \quad z \in \mathbb{C}$$

Moreover, $A \in \text{BIP}(0)$.

- (iv) Let again E_0 be a Hilbert space and assume that $-A$ is m -dissipative and satisfies $0 \in \rho(A)$. Then $A \in \text{BIP}(\pi/2)$.

Given $p \in (1, \infty)$, Sobolev’s embedding theorem ensures that $W_p^1((0, T), E_0)$ is continuously injected into $C([0, T], E_0)$. Consequently, given any function $u \in W_p^1((0, T), E_0)$ and $t \in [0, T]$, the pointwise

evaluation $u(t)$ is well defined. In particular, the trace at 0 with respect to time

$$\text{tr} : W_p^1((0, T), E_0) \rightarrow E_0, \quad u \mapsto u(0)$$

is a well-defined and bounded linear operator. In order to formulate the next result, let $E_{s,p} = (E_0, E_1)_{s,p}$, with $p \in (1, \infty)$ and $s \in (0, 1)$, denote the real interpolation space between the basic space E_0 and E_1 , the domain $D(A)$ of A , endowed with the graph norm. Furthermore, we set

$$E_0 := L_p((0, T), E_0)$$

$$E_1 := L_p((0, T), E_1) \cap W_p^1((0, T), E_0)$$

and we write $\text{Isom}(E, F)$ for the set of all topological isomorphisms mapping the Banach space E onto the Banach space F .

Theorem 8 (Dore and Venni). *Suppose that E_0 is a UMD space and that $A \in \text{BIP}(\theta)$ for some $\theta \in [0, \pi/2)$. Then, given $p \in (1, \infty)$, we have*

$$(\partial_t + A, \text{tr}) \in \text{Isom}(E_1, E_0 \times E_{1-1/p,p})$$

This means that, given $(f, u_0) \in L_p((0, T), E_0) \times E_{1-1/p,p}$, there exists a unique solution $u \in L_p((0, T), E_1) \cap W_p^1((0, T), E_0)$ of the Cauchy problem [6]. Moreover, u depends continuously on (f, u_0) and fulfills the following a priori estimate:

$$\|u\|_{E_1} \leq c(\|f\|_{E_0} + \|u_0\|_{E_{1-1/p,p}})$$

$$\text{where } c := \|(\partial_t + A, \text{tr})^{-1}\|_{\mathcal{L}(E_0 \times E_{1-1/p,p}, E_1)}.$$

Nonautonomous Equations of Hyperbolic Type

According to Theorem 1 and the corresponding remark, it is reasonable to impose in the study of the Cauchy problem [1] the minimal hypothesis that, given $s \in [0, T]$, each individual operator $A(s)$ be the generator of a C_0 -semigroup $\{T_s(t); t \geq 0\}$ in $\mathcal{L}(E_0)$. If this semigroup is holomorphic, we call [1] of “parabolic type.” Otherwise the evolution equation [1] is said to be of “hyperbolic type.”

A family $\{A(t); t \in [0, T]\}$ of generators of C_0 -semigroups in $\mathcal{L}(E_0)$ is called “stable” iff there exist positive constants M and ω such that $(\omega, \infty) \subset \rho(A(t))$ for all $t \in [0, T]$ and such that

$$\left\| \prod_{j=1}^k (\lambda - A(t_j))^{-1} \right\| \leq M(\lambda - \omega)^{-k} \quad \text{for } \lambda > \omega$$

and every finite sequence $0 \leq t_1 \leq t_2 \leq \dots \leq t_k \leq T$ with $k \in \mathbb{N}$. Observe that the resolvent operators $(\lambda - A(t_j))^{-1}$ do not commute in general. Therefore, the order of the terms on the left-hand side of the above estimate has to be obeyed. Assume that $\mathcal{A} = \{A(t); t \in [0, T]\}$ is a family of m -dissipative operators. Then, \mathcal{A}

is stable, since any m -dissipative operator B satisfies the estimate $\|(\lambda - B)^{-1}\| \leq 1/\lambda$ for all $\lambda > 0$.

It turns out that the stability of a family of generators is not sufficient to construct a solution of [1] even in the case $f \equiv 0$. We also need a certain time regularity of the mapping $t \mapsto A(t)$. For this we say that the family $\{A(t); t \in [0, T]\}$ has a common domain D iff D is a dense subspace of E_0 such that $D(A(t)) = D$ for all $t \in [0, T]$. The family $\{A(t); t \in [0, T]\}$ is called “strongly differentiable” iff it has a common domain D and, given $v \in D$, the function $t \mapsto A(t)v$ belongs to $C^1([0, T], E_0)$.

We are now prepared to formulate the following result.

Theorem 9 (Kato). *Let $\{A(t); t \in [0, T]\}$ be a stable and strongly differentiable family of generators of C_0 -semigroups with common domain D . If $f \in C^1([0, T], E_0)$ and $u_0 \in D$ then [1] possesses a unique classical solution.*

The above result is based on the construction of an evolution operator $U(t, s)$, which can be considered as the generalization of the notion of a C_0 -semigroup for autonomous equations to the case evolution equations of the form

$$u'(t) = A(t)u(t), \quad t \in (s, T], \quad u(s) = v$$

for fixed $s \in [0, T)$. Once an evolution operator is available, the solution of [1] is given by

$$u(t) = U(t, 0)u_0 + \int_0^t U(t, s)f(s) ds, \quad t \in [0, T]$$

Of course, this generalizes [7] and if $A(t)$ is independent of t , then $U(t, s) = T(t - s)$, where $\{T(t); t \geq 0\}$ is the semigroup generated by $A(0)$.

Furthermore, there are several extensions of the Kato’s result. Among them the most interesting contributions are concerned to weaken the time regularity of f and to weaken the assumption that $\{A(t); t \in [0, T]\}$ be strongly differentiable. In particular, it is possible to study [1] for families without a common domain.

For the construction of evolution operators as well as generalizations of Theorem 9, the reader is again referred to the “Further reading” section.

Nonautonomous Equations of Parabolic Type

Throughout this section we assume that E_0 and E_1 are Banach spaces such that E_1 is dense and continuously injected in E_0 . In the study of parabolic evolution equations, the class of all operators in $\mathcal{L}(E_1, E_0)$, considered as unbounded operators in E_0 with common domain E_1 , which generate holomorphic C_0 -semigroups in $\mathcal{L}(E_0)$ has turned out to

be very useful. In the following, we call this class $\mathcal{H}(E_1, E_0)$. It is known that $A \in \mathcal{H}(E_1, E_0)$ iff there exist constants $\omega > 0$ and $\kappa \geq 1$ such that $\omega - A \in \text{Isom}(E_1, E_0)$ and such that

$$\kappa^{-1} \leq \frac{\|(\lambda - A)x\|_0}{|\lambda|\|x\|_0 + \|x\|_1} \leq \kappa$$

$$x \in E_1 \setminus \{0\}, \quad \text{Re } \lambda \geq \omega$$

where $\|\cdot\|_j$ denotes the norm of E_j . Using the above characterization, it can be shown that $\mathcal{H}(E_1, E_0)$ is an open subset of $\mathcal{L}(E_1, E_0)$. In the following, we always endow $\mathcal{H}(E_1, E_0)$ with the topology induced by the norm of $\mathcal{L}(E_1, E_0)$. As a consequence of this convention it is meaningful to consider, for example, continuous mappings from $[0, T]$ into $\mathcal{H}(E_1, E_0)$. Observe that if $A \in C([0, T], \mathcal{H}(E_1, E_0))$, then $\mathcal{A} = \{A(t); t \in [0, T]\}$ is a family of generators of holomorphic semigroups with the common domain E_1 . Then we have the following result.

Theorem 10 (Sobolevskii, Tanabe). *Assume that there is a $\rho \in (0, 1)$ such that*

$$(A, f) \in C^p([0, T], \mathcal{H}(E_1, E_0) \times E_0)$$

Then, given $u_0 \in E_0$, the Cauchy problem [1] possesses a unique classical solution u . This solution has the additional regularity

$$u \in C^p((0, T], E_1) \cap C^{1+\rho}((0, T], E_0)$$

Finally, if $u_0 \in E_1$, then $u \in C^1([0, T], E_0)$.

As in the hyperbolic case, the proof of Theorem 10 is based on the evolution operator $U(t, s)$ for the homogeneous problem, although the constructions of the corresponding evolution operators are completely different.

In addition, there are several extensions and generalizations of Theorem 10. In particular, the assumption that the family $\{A(t); t \in [0, T]\}$ possesses a common domain can be weakened considerably. Furthermore, it is possible to look at parabolic evolution equations in the so-called interpolation and extrapolation scales. This offers a great flexibility in the study of nonlinear problems. Further details in this direction can be found in the "Further reading" section.

Nonlinear Evolution Equations

Let E_0, E_1 be Banach spaces such that E_1 is dense and continuously embedded in E_0 . Assume further that $u_0 \in E_1$ and that we are given a nonlinear operator $F \in C([0, T] \times V, E_0)$, where V is an open neighborhood of u_0 in E_1 . In this section, we will discuss the well-posedness of the

Cauchy problem for the following nonlinear evolution equation

$$u'(t) = F(t, u(t)), \quad t \in (0, T], \quad u(0) = u_0 \quad [9]$$

in the Banach space E_0 . We will always assume that the nonlinear operator F either carries a quasilinear structure or is of fully nonlinear parabolic type. By a "quasilinear structure," we mean that there is mapping $A \in C([0, T] \times V, \mathcal{L}(E_1, E_0))$ and a suitable "lower-order term" $f \in C([0, T] \times V, E_0)$ such that

$$F(t, v) = A(t, v)v + f(t, v)$$

$$\text{for all } (t, v) \in [0, T] \times V$$

Problem [9] is of fully nonlinear parabolic type if $F \in C^1([0, T] \times V, E_0)$ and if the Fréchet derivative $D_2 F(0, u_0)$ of F with respect to v at $(0, u_0)$ belongs to the class $\mathcal{H}(E_1, E_0)$.

Quasilinear Evolution Equations of Hyperbolic Type

Assume that E_0 is a reflexive Banach space and let $u_0 \in V \subset E_1$ be chosen as above. We consider the following abstract quasilinear evolution equation of hyperbolic type:

$$u'(t) = A(t, u(t))u(t) + f(t, u(t)), \quad t \in (0, T] \quad [10]$$

$$u(0) = u_0$$

and assume that the following hypotheses are satisfied:

(H₁) $A \in C([0, T] \times V, \mathcal{L}(E_1, E_0))$ is bounded on bounded subsets of V and, given $(t, v) \in [0, T] \times V$, the operator $A(t, v)$ is m -dissipative and there is a constant μ_A such that

$$\|A(t, v) - A(t, w)\|_{\mathcal{L}(E_1, E_0)} \leq \mu_A \|v - w\|_{E_0}$$

for all $t \in [0, T]$ and all $v, w \in V$.

(H₂) There is a $Q \in \text{Isom}(E_1, E_0)$ such that $QA(t, v)Q^{-1} = A(t, v) + B(t, v)$, where $B(t, v) \in \mathcal{L}(E_0)$ is bounded, uniformly on bounded subsets of V . Moreover,

$$\|B(t, v) - B(t, w)\|_{\mathcal{L}(E_0)} \leq \mu_B \|v - w\|_{E_1}$$

for all $t \in [0, T]$ and all $v, w \in V$.

(H₃) $f \in C([0, T] \times V, E_1)$ is bounded on bounded subsets of V and there are μ_0 and μ_1 such that

$$\|f(t, v) - f(t, w)\|_{E_j} \leq \mu_j \|v - w\|_{E_j}$$

$$\text{for all } v, w \in V, j \in \{0, 1\}$$

Then we have the following result.

Theorem 11 (Kato). *Assume that (H₁), (H₂), and (H₃) are satisfied. Then there is a maximal*

$t^+ \in (0, T]$, depending only on $\|u_0\|_{E_1}$, and a unique solution u to [10] such that

$$u = u(\cdot, u_0) \in C([0, t^+], V) \cap C^1([0, t^+], E_0)$$

Moreover, the mapping $u_0 \mapsto u(\cdot, u_0)$ is continuous from V to $C([0, t^+], V) \cap C^1([0, t^+], E_0)$.

There are many applications of Theorem 11 to different concrete partial differential equations (PDEs), including symmetric hyperbolic first-order systems, the Korteweg-de Vries equation, nonlinear elastodynamics, quasilinear wave equations, Navier-Stokes and Euler equations, and coupled Maxwell-Dirac equations. We decided to explain in some detail an application to the so-called periodic Camassa-Holm equation:

$$u_t - u_{xxt} + 3uu_x = 2u_x u_{xx} + uu_{xxx} \quad t > 0, x \in S^1 \quad [11]$$

where S^1 stands for the unit circle. In the above model, the function u is the height of a unilinear water wave over a flat bottom.

Set $X := L_2(S^1)$, $V := H^1(S^1)$, and $Q := (I - \partial_x^2)^{1/2}$. With $y := u - u_{xx}$, eqn [11] can be re-expressed as

$$y_t + (Q^{-2}y)_x = -2y(Q^{-2}y)_x \quad \text{in } L_2(S^1)$$

which is of type [10] with

$$A(y) = (Q^{-2}y)\partial_x, \quad f(y) = -2y(Q^{-2}y)_x, \quad y \in V$$

where $\text{dom}(A(y)) := \{v \in L_2(S^1); (Q^{-2}y)v \in H^1(S^1)\}$.

Quasilinear Evolution Equations of Parabolic Type

Assume that E_0 and E_1 are Banach spaces such that E_1 is dense and continuously injected in E_0 . Moreover, let $(\cdot, \cdot)_\theta$ for each $\theta \in (0, 1)$ be an admissible interpolation functor (e.g., the real or complex interpolation functor) and set $E_\theta := (E_0, E_1)_\theta$ for $\theta \in (0, 1)$. Given a subset $X \subset E_\theta$ for some $\theta \in (0, 1)$, we set $X_\eta := X \cap E_\eta$ for $\eta \in [0, 1]$, equipped with the topology induced by E_η . Finally, we write $C^{1-}(M, N)$ for the class of all locally Lipschitz continuous functions mapping the metric space M into the metric space N .

Theorem 12 (Amann). Suppose that $0 < \gamma \leq \beta < \alpha < 1$, that X_β is open in E_β , and that

$$(A, f) \in C^{1-}([0, T] \times X_\beta, \mathcal{H}(E_1, E_0) \times E_\gamma)$$

Then, given $u_0 \in X_\alpha$, there exists a unique maximal $t^+ \in (0, T]$, such that the quasilinear parabolic Cauchy problem

$$u'(t) = A(t, u(t))u(t) + f(t, u(t)), \quad t \in (0, T], \quad u(0) = u_0$$

possesses a unique classical solution

$$u := u(\cdot, u_0) \in C([0, t^+], X_\alpha) \cap C^1((0, t^+), E_0)$$

Assume A and f are independent of t and let $u(\cdot, u_0)$ be the solution to corresponding autonomous problem

$$u'(t) = A(u(t))u(t) + f(u(t)), \quad t \in (0, \infty), \quad u(0) = u_0$$

Then the mapping $(t, u_0) \mapsto u(t, u_0)$ is a semiflow on X_α .

Due to its clarity and flexibility, Theorem 12 has found a plethora of applications, which we cannot discuss in detail here. Let us at least mention the following: reaction-diffusion systems, population dynamics, phase transition models, flows through porous media, Stefan problems, and nonlinear and dynamic boundary conditions in boundary-value problems. In addition, many geometric evolution equations fall into the scope of Theorem 12. Consider, for example, the volume-preserving gradient flow of the area functional of a compact hypersurface M in \mathbb{R}^{m+1} with respect to $L_2(M)$ and $W_2^{-1}(M)$, respectively. These flows are known as the averaged mean curvature flow and the surface diffusion flow, respectively, and have been investigated on the basis of Theorem 12.

Fully Nonlinear Evolution Equations of Parabolic Type

Based on the theory of maximal regularity for linear evolution equations, it is possible to investigate abstract fully nonlinear parabolic problems of type [9]. As there are different techniques of maximal regularity, there are also different approaches to [9]. We present here a result which uses maximal regularity properties in singular Hölder spaces C_β^β . Let E_0 and E_1 be Banach spaces such that E_1 is continuously embedded into E_0 (density of E_1 in E_0 is not needed here). As before, V is an open subset of E_1 and D_2F stands for the Fréchet derivative of $F(t, v)$ with respect to the second variable.

Theorem 13 (Lunardi). Assume that $F \in C^2([0, T] \times V, E_0)$ such that $D_2F \in C^1([0, T] \times V, \mathcal{H}(E_1, E_0))$. Then, given $u_0 \in V$, there is a maximal $t^+ \in (0, T]$ such that problem [9] has a solution $u \in C([0, t^+], E_1) \cap C^1([0, t^+], E_0)$. This solution is unique in the class

$$\bigcup_{0 < \beta < 1} C_\beta^\beta((0, t^+ - \varepsilon], E_1) \cap C([0, t^+ - \varepsilon], E_1)$$

for each $\varepsilon \in (0, t^+)$.

Theorem 13 has important applications to problems for which the hypotheses of Theorem 12 (in particular the assumption on the quasilinear structure) are not

satisfied. We mention here fully nonlinear second-order boundary-value problems, Hele–Shaw models, models from combustion theory, and Bellman equations.

See also: Boltzmann Equation (Classical and Quantum); Breaking Water Waves; Dissipative Dynamical Systems of Infinite Dimension; Elliptic Differential Equations: Linear Theory; Ginzburg–Landau Equation; Image Processing: Mathematics; Incompressible Euler Equations: Mathematical Theory; Nonlinear Schrödinger Equations; Partial Differential Equations: Some Examples; Quantum Dynamical Semigroups; Relativistic Wave Equations Including Higher Spin Fields; Semilinear Wave Equations; Separation of Variables for Differential Equations; Singularities of the Ricci Flow; Symmetric Hyperbolic Systems and Shock Waves; Wave Equations and Diffraction.

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Exact Renormalization Group

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Introduction

The renormalization group (RG) in its modern form was invented by K G Wilson in the context of statistical mechanics and Euclidean quantum field theory (EQFT). It offers the deepest understanding of renormalization in quantum field theory (QFT) by connecting EQFT with the theory of second-order phase transition and associated critical phenomena. Thermodynamic functions of many statistical mechanical models (the prototype being the Ising model in two or more dimensions) exhibit power-like singularities as the temperature approaches a critical value. One of the major triumphs of the Wilson RG was the prediction of the exponents (known as critical exponents) associated to these singularities. Wilson's fundamental contribution was to realize that many length scales begin to cooperate as one approaches criticality and that one should disentangle them and treat them one at a time. This leads to an iterative procedure known as the “renormalization group.” Singularities and critical exponents then arise from a limiting process.

Ultraviolet singularities of field theory can also be understood in the same way. Wilson reviews this (Wilson and Kogut 1974) and gives the historical genesis of his ideas (Wilson 1983).

The early work in the subject was heuristic, in the sense that clever but uncontrolled approximations were made to the exact equations often with much success. Subsequently, authors with mathematical bent began to use the underlying ideas to prove theorems. Benfatto, Cassandro, Gallavotti, Nicolo, Olivieri *et al.* pioneered the rigorous use of Wilson's renormalization group in the construction of super-renormalizable QFTs, (see Benfatto and Gallavotti (1995) and references therein). The subject saw further mathematical development in the work of Gawedzki and Kupiainen (1984, 1986) and that of Bałaban (1982), and references therein. Bałaban in a series of papers ending in Bałaban (1989) proved a basic result on the continuum limit of Wilson's lattice gauge theory. Brydges and Yau (1990) simplified the mathematical treatment of the renormalization group for a class of models and this has led to further systemization and simplification in the work of Brydges *et al.* (1998, 2003). Another method which has been intensely developed during the same historical period is based on phase cell expansions: Feldman, Magnen, Rivasseau, and Sénéor developed the early phase cell ideas of

Glimm and Jaffe and were able to prove independently many of the results cited earlier (see Rivasseau (1991) and references therein). Although these methods share many features of the Wilson RG, they are different in methodology and thus remain outside of the purview of the present exposition.

A somewhat different line of development has been the use of the RG to give simple proofs of perturbative renormalizability of various QFTs: Gallavotti and Nicolò, via iterative methods (see Benfatto and Gallavotti (1995) and references therein), and Polchinski (1984), who exploited a continuous version of the RG for which Wilson (1974) had derived a nonlinear differential equation. These early works were devoted to the standard $(\phi^4)_4$ scalar field theory, but subsequently Polchinski's work has been extended to a large class of models, including four-dimensional nonabelian gauge theories (see Kopper and Muller (2000) and references therein).

Finally, it should be mentioned that apart from QFT and statistical mechanics, the RG method has proved fruitful in other domains. An example is the study of interacting fermion systems in condensed matter physics (see Fermionic Systems and Renormalization: Statistical Mechanics and Condensed Matter). In the rest of this article, our focus will be on EQFT and statistical mechanics.

The RG as a Discrete Semigroup

We will first define a discrete version of the RG and consider its continuous version later. As we will see, the RG is really a semigroup, so calling it a group is a misnomer.

Let ϕ be a Gaussian random field (see, e.g., Gelfand and Vilenkin (1964) for a discussion of random fields) in \mathbf{R}^d . Associated to it there is a positive-definite function which is identified as its covariance. In QFT one is interested in the covariance

$$\begin{aligned} E(\phi(x)\phi(y)) &= \text{const. } |x-y|^{-2[\phi]} \\ &= \int_{\mathbf{R}^d} dp e^{ip \cdot (x-y)} \frac{1}{|p|^{d-2[\phi]}} \end{aligned} \quad [1]$$

Here $[\phi] > 0$ is the (canonical) dimension of the field, which for the standard massless free field is $[\phi] = (d-2)/2$. The latter is positive for $d > 2$. However, other choices are possible but in EQFT they are restricted by the Osterwalder-Schrader positivity. It is assured if $[\phi] = (d-\alpha)/2$, with $0 < \alpha \leq 2$. If $\alpha < 2$, we get a generalized free field.

Observe that the covariance is singular for $x = y$ and this singularity is responsible for the ultraviolet divergences of QFT. This singularity has to be initially cut off and there are many ways to do this. A simple

way is as follows. Let $u(x)$ be a smooth, rotationally invariant, positive-definite function of fast decrease. Examples of such functions are legion. Observe that

$$|x-y|^{-2\phi} = \text{const.} \int_0^\infty \frac{dl}{l} l^{-2[\phi]} u\left(\frac{x-y}{l}\right) \quad [2]$$

as can be seen by scaling in l . We define the unit ultraviolet cutoff covariance C by cutting off at the lower end point of the l integration (responsible for the singularity at $x = y$) at $l = 1$,

$$C(x-y) = \int_1^\infty \frac{dl}{l} l^{-2[\phi]} u\left(\frac{x-y}{l}\right) \quad [3]$$

$C(x-y)$ is positive-definite and everywhere smooth. Being positive-definite, it qualifies as the covariance of a Gaussian probability measure denoted μ_C on a function space Ω (which it is not necessary to specify any further). The covariance C being smooth implies that the sample fields of the measure are μ_C almost everywhere sufficiently differentiable.

Remark Note that, more generally, we could have cut off the lower end point singularity in [1] at any $\epsilon > 0$. The ϵ -cutoff covariance is related to the unit cutoff covariance by a scale transformation (defined below) and we will exploit this relation later.

Let $L > 1$ be any real number. We define a scale transformation S_L on fields ϕ by

$$S_L \phi(x) = L^{-[\phi]} \phi\left(\frac{x}{L}\right) \quad [4]$$

on covariances by

$$S_L C(x-y) = L^{-2[\phi]} C\left(\frac{x-y}{L}\right) \quad [5]$$

and on functions of fields $F(\phi)$ by

$$S_L F(\phi) = F(S_L \phi) \quad [6]$$

The scale transformations form a multiplicative group: $S_L^n = S_{L^n}$.

Now define a fluctuation covariance Γ_L :

$$\Gamma_L(x-y) = \int_1^L \frac{dl}{l} l^{-2[\phi]} u\left(\frac{x-y}{l}\right) \quad [7]$$

$\Gamma_L(x-y)$ is smooth, positive-definite and of fast decrease on scale L . It generates a key scaling decomposition

$$C(x-y) = \Gamma_L(x-y) + S_L C(x-y) \quad [8]$$

Iterating this, we get

$$C(x-y) = \sum_{n=0}^{\infty} \Gamma_n(x-y) \quad [9]$$

where

$$\Gamma_n(x-y) = S_{L^n} \Gamma_L(x-y) = L^{-2n[\phi]} \Gamma_L\left(\frac{x-y}{L^n}\right) \quad [10]$$

The functions $\Gamma_n(x-y)$ are of fast decrease on scale L^{n+1} .

Thus, [9] achieves the decomposition into a sum over increasing length scales as desired. Being positive definite, Γ_n qualify as covariances of Gaussian probability measures, and therefore $\mu_C = \bigotimes_{n=0}^{\infty} \mu_{\Gamma_n}$. Correspondingly introduce a family of independent Gaussian random fields ζ_n , called fluctuation fields, distributed according to μ_{Γ_n} . Then

$$\phi = \sum_{n=0}^{\infty} \zeta_n \quad [11]$$

Note that the fluctuation fields ζ_n are slowly varying over length scales L^n . In fact, an easy estimate using a Tchebycheff inequality shows that, for any $\gamma > 0$,

$$|x-y| \leq L^n \Rightarrow \mu_C(|\zeta_n(x) - \zeta_n(y)| \geq \gamma) \leq \text{const. } \gamma^{-2} \quad [12]$$

which reveals the slowly varying nature of ζ_n on scale L^n . Equation [11] is an example of a multiscale decomposition of a Gaussian random field.

The above implies that the μ_C integral of a function can be written as a multiple integral over the fields ζ_n . We calculate it by integrating out the fluctuation fields ζ_n step by step, going from shorter to longer length scales. This can be accomplished by the iteration of a single transformation T_L , a renormalization group transformation, as follows. Let $F(\phi)$ be a function of fields. Then we define a RG transformation $F \rightarrow T_L F$ by

$$\begin{aligned} (T_L F)(\phi) &= S_L \mu_{\Gamma_L} * F(\phi) \\ &= \int d\mu_{\Gamma_L}(\zeta) F(\zeta + S_L \phi) \end{aligned} \quad [13]$$

Thus the renormalization group transformation consists of a convolution with the fluctuation measure followed by a rescaling.

Semigroup Property

The discrete RG transformations form a semigroup:

$$T_L T_{L^n} = T_{L^{n+1}} \quad \text{for all } n \geq 0 \quad [14]$$

To prove this, we must first see how scaling commutes with convolution with a measure. We have the property

$$\mu_{\Gamma_L} * S_L F = S_L \mu_{S_L \Gamma_L} * F \quad [15]$$

To see this, observe first that if ζ is a Gaussian random field distributed with covariance Γ_L then the

Gaussian field $S_L \zeta$ is distributed according to $S_L \Gamma_L$. This can be checked by computing the covariance of $S_L \zeta$. Now the left-hand side of [15] is just the integral of $F(S_L \zeta + S_L \phi)$ with respect to $d\mu_{\Gamma_L}(\zeta)$. By the previous observation, this is the integral of $F(\zeta + S_L \phi)$ with respect to $d\mu_{S_L \Gamma_L}(\zeta)$, and the latter is the right-hand side of [15]. Now we can check the semigroup property trivially:

$$\begin{aligned} T_L T_{L^n} F &= S_L \mu_{\Gamma_L} * S_{L^n} \mu_{\Gamma_{L^n}} * F \\ &= S_L S_{L^n} \mu_{S_{L^n} \Gamma_{L^n}} * \mu_{\Gamma_{L^n}} * F \\ &= S_{L^{n+1}} \mu_{\Gamma_{L^n} + S_{L^n} \Gamma_L} * F \\ &= S_{L^{n+1}} \mu_{\Gamma_{L^{n+1}}} * F \\ &= T_{L^{n+1}} F \end{aligned} \quad [16]$$

We have used the fact that $\Gamma_{L^n} + S_{L^n} \Gamma_L = \Gamma_{L^{n+1}}$. This is because $S_{L^n} \Gamma_L$ has the representation [7] with integration interval changed to $[L^n, L^{n+1}]$.

We note some properties of T_L . T_L has an unique invariant measure, namely μ_C : for any bounded function F ,

$$\int d\mu_C T_L F = \int d\mu_C F \quad [17]$$

To understand [17], recall the earlier observation that if ϕ is distributed according to the covariance C , then $S_L \phi$ is distributed according to $S_L C$. By [8], $\Gamma_L + S_L C = C$. Therefore,

$$\begin{aligned} \int d\mu_C T_L F &= \int d\mu_C S_L \mu_{\Gamma_L} * F \\ &= \int d\mu_{S_L C} \mu_{\Gamma_L} * F \\ &= \int d\mu_C F \end{aligned} \quad [18]$$

The uniqueness of the invariant measure follows from the fact that the semigroup T_L is realized by a convolution with a probability measure and, therefore, is positivity improving:

$$F \geq 0, \mu_C \text{ a.e.} \Rightarrow T_L F > 0, \mu_C \text{ a.e.}$$

Finally, note that T_L is a contraction semigroup on $L^p(d\mu_C)$ for $1 \leq p < \infty$. To see this, note that since T_L is a convolution with a probability measure $T_L F = \mu_{S_{L^{-1}} \Gamma_L} * S_L F$, we have, via Hölder's inequality, $|T_L F|^p \leq T_L |F|^p$. Then use the fact that μ_C is an invariant measure.

Eigenfunctions

Let $:p_{n,m}:(\phi(x))$ be a C Wick-ordered local monomial of m fields with n derivatives. Define

$$P_{n,m}(X) = \int_X dx :p_{n,m}:_C(x)$$

The functions $P_{n,m}(X)$ play the role of eigenfunctions of the RG transformation T_L up to a scaling of volume:

$$T_L P_{n,m}(X) = L^{d-m[\phi]-n} P_{n,m}(L^{-1}X) \quad [19]$$

Because of the scaling in volume, $P_{n,m}(X)$ are not true eigenfunctions. Nevertheless, they are very useful because they play an important role in the analysis of the evolution of the dynamical system which we will later associate with T_L . They are classified as expanding (relevant), contracting (irrelevant) or central (marginal), depending on whether the exponent of L on the right-hand side of [19] is positive, negative, or zero, respectively. This depends, of course, on the space dimension d and the field dimension $[\phi]$.

Gaussian measures are of limited interest. But we can create new measures by perturbing the Gaussian measure μ_C with local interactions. We cannot study directly the situation where the interactions are in infinite volume. Instead, we put them in a very large volume which will eventually go to infinity. We have a ratio of two length scales, one from the size of the diameter of the volume and the other from the ultraviolet cutoff in μ_C , and this ratio is enormous. The RG is useful whenever there are two length scales whose ratio is very large. It permits us to do a scale-by-scale analysis and at each step the volume is reduced at the cost of changing the interactions. The largeness of the ratio is reflected in the large number of steps to be accomplished, this number tending eventually to infinity. This large number of steps has to be controlled mathematically.

Perturbation of the Gaussian Measure

Let $\Lambda_N = [-L^N/2, L^N/2]^d \subset \mathbf{R}^d$ be a large cube in \mathbf{R}^d . For any $X \subset \Lambda_N$, let $V_0(X, \phi)$ be a local semibounded function where the fields are restricted to the set X . Here “local” means that if X, Y are sets with disjoint interiors then $V_0(X \cup Y, \phi) = V_0(X) + V_0(Y)$. Consider the integral (known as the partition function in QFT and statistical mechanics)

$$Z(\Lambda_N) = \int d\mu_C(\phi) z_0(\Lambda_N, \phi) \quad [20]$$

where

$$z_0(X, \phi) = e^{-V_0(X, \phi)} \quad [21]$$

and

$$d\mu^{(0)}(\Lambda_N, \phi) = \frac{1}{Z(\Lambda_N)} d\mu_C(\phi) e^{-V_0(\Lambda_N, \phi)} \quad [22]$$

is the corresponding probability measure. V_0 is typically not quadratic in the fields and therefore leads to a non-Gaussian perturbation. For example,

$$V_0(X, \phi) = \int_X dx (\xi |\nabla \phi(x)|^2 + g_0 \phi^4(x) + \mu_0 \phi^2(x)) \quad [23]$$

where we take $g_0 > 0$. The integral [20] is well defined because the sample fields are smooth.

We now proceed to the scale-by-scale analysis mentioned earlier. Because μ_C is an invariant measure of T_L , we have the partition function $Z(\Lambda_N)$ in the volume Λ_N as

$$\begin{aligned} Z(\Lambda_N) &= \int d\mu_C(\phi) z_0(\Lambda_N, \phi) \\ &= \int d\mu_C(\phi) T_L z_0(\Lambda_N, \phi) \end{aligned} \quad [24]$$

The integrand on the right-hand side is a new function of fields which, because of the final scaling, live in the smaller volume Λ_{N-1} . This leads to the following definition:

$$z_1(\Lambda_{N-1}, \phi) = T_L z_0(\Lambda_N, \phi) \quad [25]$$

Because V_0 is local, z_0 has a factorization property for unions of sets with disjoint interiors. This is no longer the case for z_1 . Wilson noted that, nevertheless, the integral is well approximated by an integrand which does, but the approximator has new coupling constants. The phrase “well approximated” is what all the rigorous work is about and this was not evident in the early Wilson era. The idea is to extract out a local part and also consider the remainder. The local part leads to a flow of coupling constants and the (unexponentiated) remainder is an irrelevant term. This operation and its mathematical control is an essential feature of RG analysis.

Iterating the above transformation, we get, for all $0 \leq n \leq N$,

$$z_{n+1}(\Lambda_{N-n-1}, \phi) = T_L z_n(\Lambda_{N-n}, \phi) \quad [26]$$

After N iterations, we get

$$Z(\Lambda_N) = \int d\mu_C(\phi) z_N(\Lambda_0, \phi) \quad [27]$$

where Λ_0 is the unit cube. To take the limit as $N \rightarrow \infty$, we have to control the infinite sequence of iterations. We cannot hope to control the infinite sequence at the level of the entire partition function. Instead, one chooses representative coordinates for which the infinite sequence has a chance of having a meaning. The coordinates are provided by the coupling constants of the extracted local part and the irrelevant terms (an

approximate calculation of the flow of coupling constants is given in the next section). The existence of a global trajectory for such coordinates helps us to control the limit for moments of the probability measure (correlation functions). The question of coordinates and the representation of the irrelevant terms will be taken up in the section “Rigorous RG analysis.”

Ultraviolet Cutoff Removal

The next issue is ultraviolet cutoff removal in field theory. This problem can be put into the earlier framework as follows. Let ϵ_N be a sequence of positive numbers which tend to 0 as $N \rightarrow \infty$. Following the remark after [3], we replace the unit cutoff covariance C by the covariance C_{ϵ_N} defined by taking ϵ_N (instead of 1) as the lower end point in the integral [3]. Thus, ϵ_N acts as a short-distance or ultraviolet cutoff. It is easy to see that

$$C_{\epsilon_N}(x - y) = S_{\epsilon_N} C(x - y) \quad [28]$$

Consider the partition function, $Z_{\epsilon_N}(\Lambda)$ in a cube $\Lambda = [-R/2, R/2]^d$:

$$Z_{\epsilon_N}(\Lambda) = \int d\mu_{C_{\epsilon_N}}(\phi) e^{-V_0(\Lambda, \phi, \tilde{\xi}_N, \tilde{g}_N, \tilde{\mu}_N)} \quad [29]$$

where V_0 is given by [23] with g_0, μ_0 replaced by $\tilde{g}_N, \tilde{\mu}_N$, respectively. By dimensional analysis we can write

$$\begin{aligned} \tilde{\xi}_N &= \epsilon_N^{(2[\phi]-d+2)} \xi, & \tilde{g}_N &= \epsilon_N^{(4[\phi]-d)} g, \\ \tilde{\mu}_N &= \epsilon_N^{(2[\phi]-d)} \mu \end{aligned} \quad [30]$$

where g, ξ, μ are dimensionless parameters. Now ϕ distributed according to C_{ϵ_N} equals in distribution $S_{\epsilon_N} \phi$ distributed according to C . Therefore, choosing $\epsilon_N = L^{-N}$, we get

$$\begin{aligned} Z_{\epsilon_N}(\Lambda) &= \int d\mu_C(\phi) e^{-V_0(\Lambda, S_{\epsilon_N} \phi, \tilde{\xi}_N, \tilde{g}_N, \tilde{\mu}_N)} \\ &= \int d\mu_C(\phi) e^{-V_0(\Lambda_N, \phi, \xi g, \mu)} \end{aligned} \quad [31]$$

where $\Lambda_N = [-L^N R/2, L^N R/2]^d$. Thus, the field theory problem of removing the ultraviolet cutoff, that is, taking the limit $\epsilon_N \rightarrow 0$, has been reduced to the study of a statistical mechanical model in a very large volume. The latter has to be analyzed via RG iterations as before.

Critical Field Theories

As mentioned earlier, we have to study the flow of local interactions as well as that of irrelevant terms. Together they constitute the RG trajectory and we have to prove that it exists globally. In general, the

trajectory will tend to explode after a large number of iterations due to growing relevant terms (characterized in terms of the expanding Wick monomials mentioned earlier). Wilson pointed out that the saving factor is to exploit fixed points and their invariant manifolds by tuning the initial interaction so that the RG has a global trajectory. This leads to the notion of a critical manifold which can be defined as follows. A fixed point will have contracting and/or marginal attractive directions besides the expanding ones. In the language of dynamical systems, the critical manifold is the stable or center stable manifold of the fixed point in question. This is determined by a detailed study of the discrete flow. In the examples above, it amounts to fixing the initial “mass” parameter $\mu_0 = \mu_c(g_0)$ with a suitable function μ_c such that the flow remains bounded in an invariant set. The critical manifold is then the graph of a function from the space of contracting and marginal variables to the space of μ ’s which remains invariant under the flow. Restricted to it the flow will now converge to a fixed point. All references to initial coupling constants have disappeared. The result is known as a critical theory.

Critical theories have been rigorously constructed in a number of cases. Take the standard ϕ^4 in d dimensions. Then $[\phi] = (d - 2)/2$. For $d > 5$ the ϕ^4 interaction is irrelevant and the Gaussian fixed point is attractive with one unstable direction (corresponding to μ). In this case one can prove that the interactions converge exponentially fast to the Gaussian fixed point on the critical manifold. For $d = 4$ the interaction is marginal and the Gaussian fixed point attractive for $g > 0$. The critical theory has been constructed by Gawedzki and Kupainen (1984) starting with a sufficiently small coupling constant. The fixed point is Gaussian (interactions vanish in the limit) and the convergence rate is logarithmic. This is thus a mean-field theory with logarithmic corrections, as expected on heuristic grounds. The mathematical construction of the critical theory in $d = 3$ is an open problem. (It is expected to exist with a non-Gaussian fixed point, and this is indicated by the perturbative ϵ expansion of Wilson and Fisher in $4 - \epsilon$ dimensions.) However, the critical theory for $d = 3$ for $[\phi] = (3 - \epsilon)/4$ for $\epsilon > 0$ held very small has been rigorously constructed by Brydges *et al.* (2003). This theory has a nontrivial hyperbolic fixed point of $O(\epsilon)$. The stable manifold is constructed in a small neighborhood of the fixed point. Note that the covariance without cutoff is Osterwalder–Schrader positive and thus this is a candidate for a nontrivial EQFT. For $\epsilon = 1$ we have the standard situation in $d = 3$, and

this remains open, as mentioned earlier. A very simplified picture of the above is furnished by the perturbative computation in the next section.

Unstable Fixed Points

We may attempt to construct field theories around unstable fixed points. In this case the initial parameters have to be adjusted as functions of the cutoff in such a way as to stabilize the flow in the neighborhood of the fixed point. This may be called a genuine renormalization. A famous example of this is pure Yang–Mills theory in $d=4$, where the Gaussian fixed point has only marginal unstable directions. Balaban in a series of papers ending in Balaban (1989) considered Wilson’s lattice cutoff version of Yang–Mills theory in $d=4$ with initial coupling fixed by the two-loop asymptotic freedom formula. He proved, by lattice RG iterations, that in the weak-coupling regime the free energy per unit volume is bounded above and below by constants independent of the lattice spacing. Instability of the flow is expected to lead to mass generation for observables but this is a famous open problem. Another example is the standard nonlinear sigma model for $d=2$. Here too the flow is unstable around the Gaussian fixed point and we can set the initial coupling constant by the two-loop asymptotic freedom formula. Although much is known via approximation methods (as well as by methods based on integrable systems) this theory remains to be rigorously constructed as an EQFT.

Let us now consider a relatively simpler example, that of constructing a massive super-renormalizable scalar field theory. This has been studied in $d=3$, with $[\phi]=(d-2)/2=1/2$. We get $\xi=\tilde{\xi}$, $g=L^{-N}\tilde{g}$, $\mu=L^{-2N}\tilde{\mu}$, and \tilde{g} is taken to be small. ξ is marginal, whereas g, μ are relevant parameters and grow with the iterations. After N iterations, they are brought up to $\tilde{g}, \tilde{\mu}$ together with remainders. This realizes the so-called massive continuum ϕ^4 theory in $d=3$, and this has been mathematically controlled in the exact RG framework. This was proved by Brydges, Dimock, and Hurd and earlier by Benfatto, Cassandro, Gallavotti, and others, (see the references in Brydges *et al.* (1998) and Benfatto and Gallavotti (1995)).

The Exact RG as a Continuous Semigroup

The discrete semigroup defined in [13] of the previous section has a natural continuous counterpart. Just take L to be a continuous parameter, $L=e^t$, $t \geq 0$, and

write by abuse of notation T_t, S_t, Γ_t instead of T_{e^t} , etc. The continuous transformations T_t ,

$$T_t F = S_t \mu_{\Gamma_t} * F \quad [32]$$

give a semigroup

$$T_t T_s = T_{t+s} \quad [33]$$

of contractions on $L^2(d\mu_C)$ with μ_C as invariant measure. One can show that T_t is strongly continuous and, therefore, has a generator which we will call \mathcal{L} . This is defined by

$$\mathcal{L}F = \lim_{t \rightarrow 0^+} \frac{T_t - 1}{t} F \quad [34]$$

whenever this limit exists. This restricts F to a suitable subspace $\mathcal{D}(\mathcal{L}) \subset L^2(d\mu_C)$. $\mathcal{D}(\mathcal{L})$ contains, for example, polynomials in fields as well as twice-differentiable bounded cylindrical functions. The generator \mathcal{L} can be easily computed. To state it, we need some definitions. Define $(D^n F)(\phi; f_1, \dots, f_n)$ as the n th tangent map at ϕ along directions f_1, \dots, f_n . The functional Laplacian Δ_{Γ} is defined by

$$\Delta_{\Gamma} F(\phi) = \int d\mu_{\Gamma}(\zeta) (D^2 F)(\phi; \zeta, \zeta) \quad [35]$$

where $\dot{\Gamma} = u$. Define an infinitesimal dilatation operator

$$\mathcal{D}\phi(x) = x \cdot \nabla \phi(x) \quad [36]$$

and a vector field \mathcal{X} ,

$$\mathcal{X}F = -[\phi](DF)(\phi; \phi) - (DF)(\phi; \mathcal{D}\phi) \quad [37]$$

Then, an easy computation gives

$$\mathcal{L} = \frac{1}{2} \Delta_{\Gamma} + \mathcal{X} \quad [38]$$

T_t is a semigroup with \mathcal{L} as generator. Therefore, $T_t = e^{t\mathcal{L}}$. Let $F_t(\phi) = T_t F(\phi)$. Then F_t satisfies the linear PDE

$$\frac{\partial F_t}{\partial t} = \mathcal{L}F_t \quad [39]$$

with the initial condition $F_0 = F$. This evolution equation assumes a more familiar form if we write $F_t = e^{-V_t}$, V_t being known as the effective potential. We get

$$\frac{\partial V_t}{\partial t} = \mathcal{L}V_t - \frac{1}{2} (V_t)_{\phi} \cdot (V_t)_{\phi} \quad [40]$$

where

$$(V_t(\phi))_{\phi} \cdot (V_t(\phi))_{\phi} = \int d\mu_{\Gamma}(\zeta) ((DV_t)(\phi; \zeta))^2 \quad [41]$$

and $V_0 = V$. This infinite-dimensional nonlinear PDE is a version of Wilson’s flow equation. Note that the linear semigroup T_t acting on

functions induces a semigroup \mathcal{R}_t acting non-linearly on effective potentials giving a trajectory $V_t = \mathcal{R}_t V_0$.

Equations like the above are notoriously difficult to control rigorously, especially for large times. However, they may be solved in formal perturbation theory when the initial V_0 is small via the presence of small parameters. In particular, they give rise easily to perturbative flow equations for coupling constants. They can be obtained to any order but then there is the remainder. It is hard to control the remainder from the flow equation for effective potentials in bosonic field theories. They require other methods based on the discrete RG. Nevertheless, these approximate perturbative flows are very useful for getting a preliminary view of the flow. Moreover, their discrete versions figure as an input in further nonperturbative analysis.

Perturbative Flow

It is instructive to see this in second-order perturbation theory. We will simplify by working in infinite volume (no infrared divergences can arise because $\dot{\Gamma}(x-y)$ is of fast decrease). Now suppose that we are in standard ϕ^4 theory with $[\phi] = (d-2)/2$ and $d > 2$. We want to show that

$$V_t = \int dx \left(\xi_t : |\nabla \phi(x)|^2 : + g_t : \phi(x)^4 : + \mu_t : \phi(x)^2 : \right) \quad [42]$$

satisfies the flow equation in second order modulo irrelevant terms provided the parameters flow correctly. We will ignore field-independent terms. The Wick ordering is with respect to the covariance C of the invariant measure. The reader will notice that we have ignored a ϕ^6 term which is actually relevant in $d=3$ for the above choice of $[\phi]$. This is because we will only discuss the $d=3$ case for the model discussed at the end of this section and for this case the ϕ^6 term is irrelevant. We will assume that ξ_t, μ_t are of order $O(g^2)$. Plug in the above in the flow equation. The quantity $\lambda_t^{n,m} : P_{n,m} :$ represents one of the terms above with m fields and n derivatives. Because \mathcal{L} is the generator of the semigroup T_t we have

$$\left(\frac{\partial}{\partial t} - \mathcal{L} \right) \lambda_t^{n,m} : P_{n,m} : = \left(\frac{d\lambda_t^{n,m}}{dt} - (d - m[\phi] - n) \lambda_t^{n,m} \right) : P_{n,m} : \quad [43]$$

Next turn to the nonlinear term in the flow equation and insert the ϕ^4 term (the others are already of order $O(g^2)$). This produces a double integral of

$\dot{\Gamma}(x-y) : \phi(x)^3 : : \phi(y)^3 :$, which after complete Wick ordering, gives

$$\begin{aligned} & -\frac{g_t^2}{2} 16 \int dx dy \dot{\Gamma}(x-y) \left(: \phi(x)^3 \phi(y)^3 : \right. \\ & \quad + 9C(x-y) : \phi(x)^2 \phi(y)^2 : + 36C(x-y) : \phi(x) \phi(y) : \\ & \quad \left. + 6C(x-y)^2 \right) \end{aligned} \quad [44]$$

Consider the nonlocal ϕ^4 term. We can localize it by writing

$$\begin{aligned} : \phi(x)^2 \phi(y)^2 : &= \frac{1}{2} : \left(\phi(x)^4 + \phi(y)^4 \right. \\ & \quad \left. - (\phi(x)^2 - \phi(y)^2)^2 \right) : \end{aligned} \quad [45]$$

The local part gives a ϕ^4 contribution and the last term above gives rise to an irrelevant contribution because it produces additional derivatives. The coefficients are well defined because $C, \dot{\Gamma}$ are smooth and $\dot{\Gamma}(x-y)$ is of fast decrease. Now the nonlocal ϕ^2 term is similarly localized. It gives a relevant local ϕ^2 contribution as well as a marginal $|\nabla \phi|^2$ contribution. Finally, the same principle applies to the nonlocal ϕ^6 contribution and gives rise to further irrelevant terms. Then it is easy to see by matching that the flow equation is satisfied in second order up to irrelevant terms (these would have to be compensated by adding additional terms in V_t) provided

$$\begin{aligned} \frac{dg_t}{dt} &= (4-d)g_t - ag_t^2 + O(g_t^3) \\ \frac{d\mu_t}{dt} &= 2\mu_t - bg_t^2 + O(g_t^3) \\ \frac{d\xi_t}{dt} &= cg_t^2 + O(g_t^3) \end{aligned} \quad [46]$$

where a, b, c are positive constants. We see from the above formulas that, up to second order in g^2 , as $t \rightarrow \infty, g_t \rightarrow 0$ for $d \geq 4$. In fact, for $d \geq 5$ the decay rate is $O(e^{-t})$ and for $d=4$ the rate is $O(t^{-1})$. However, to see if V_t converges, we also have to discuss the μ_t, ξ_t flows. It is clear that in general the μ_t flow will diverge. This is fixed by choosing the initial μ_0 to be the bare critical mass. This is obtained by integrating up to time t and then expressing μ_0 as a function of the entire g trajectory up to time t . Assume that μ_t is uniformly bounded and take $t \rightarrow \infty$. This gives the critical mass as

$$\mu_0 = b \int_0^\infty ds e^{-2s} g_s^2 = \mu_c(g_0) \quad [47]$$

This integral converges for all cases discussed above. With this choice of μ_0 we get

$$\mu_t = b \int_0^\infty ds e^{-2s} g_{s+t}^2 \quad [48]$$

and this exists for all t and converges as $t \rightarrow \infty$. Now consider the perturbative ξ flow. It is easy to see from the above that for $d \geq 4$, ξ_t converges as $t \rightarrow \infty$.

We have not discussed the $d=3$ case because the perturbative g fixed point is of order $O(1)$. But suppose we take, in the $d=3$ case, $[\phi] = (3 - \epsilon)/4$ with $\epsilon > 0$ held small as in Brydges *et al.* (2003). Then the above perturbative flow equations are easily modified (by taking account of [43]) and we get, to second order, an attractive fixed point $g_* = O(\epsilon)$ of the g flow. The critical bare mass μ_0 can be determined as before and the ξ_t flow converges. The qualitative picture obtained above has a rigorous justification.

Rigorous RG Analysis

We will give a brief introduction to rigorous RG analysis in the discrete setup in the section “The RG as a Discrete Semigroup” concentrating on the principal problems encountered and how one attempts to solve them. Our approach is borrowed from Brydges *et al.* (2003). It is a simplification of the methods initiated by Brydges and Yau in (1990) and developed further by Brydges *et al.* (1998). The reader will find other approaches to rigorous RG methods in the selected references, such as those of Balaban, Gawedzki and Kupiainen, Gallavotti, and others. We will take as a concrete example the scalar field model introduced earlier.

At the core of the analysis is the choice of good coordinates for the partition function density, z , of the section “The RG as a Discrete Semigroup”. This is provided by a polymer representation (defined below) which parametrizes z by a couple (V, K) , where V is a local potential and K is a set function also depending on the fields. Then the RG transformation T_L maps (V, K) to a new (V, K) . (V, K) remain good coordinates as the volume tends to ∞ , whereas $z(\text{volume})$ diverges. There exist norms which are suited to the fixed-point analysis of (V, K) to new (V, K) . Now comes the important point: z does not uniquely specify the representation (V, K) . Therefore, we can take advantage of this nonuniqueness to keep K small in norm and let most of the action of T_L reside in V . This process is called extraction in Brydges *et al.* (2003). It makes sure that K is an irrelevant term, whereas the local flow of V gives rise to discrete flow equations in coupling constants. We will not discuss extraction any further. In the following, we introduce the polymer representation and explain how the RG transformation acts on it.

To proceed further, we first introduce a simplification in the setup used in the section “The RG as a Discrete Semigroup.” Recall that the function u introduced in [3] was smooth, positive definite, and of rapid decrease. We will simplify further by imposing the stronger property that it is actually of finite range: $u(x) = 0$ for $|x| \geq 1$. We say that u is of finite range 1. It is easy to construct such functions. For example, if g is any smooth function of finite range $1/2$, then $u = g * g$ is a smooth positive-definite function of finite range 1. This implies that the fluctuation covariance Γ_L of [7] has finite range L . As a result, Γ_n in [10] has finite range L^{n+1} and the corresponding fluctuation fields $\zeta_n(x)$ and $\zeta_n(y)$ are independent when $|x - y| \geq L^{n+1}$.

Polymer Representation

Pave \mathbb{R}^d with closed cubes of side length 1 called 1-blocks or unit blocks denoted by Δ , and suppose that Λ is a large cube consisting of unit blocks. A connected polymer $X \subset \Lambda$ is a closed connected subset of these unit blocks. A polymer activity $K(X, \phi)$ is a map $X, \phi \rightarrow \mathbb{R}$ where the fields ϕ depend only on the points of X . We will set $K(X, \phi) = 0$ if X is not connected. A generic form of the partition function density $z(\Lambda, \phi)$ after a certain number of RG iterations is

$$z(\Lambda) = \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{X_1, \dots, X_N} e^{-V(X_c)} \prod_{j=1}^N K(X_j) \quad [49]$$

Here $X_j \subset \Lambda$ are disjoint polymers, $X = \bigcup X_j$, and $X_c = \Lambda \setminus X$. V is a local potential of the form [23] with parameters ξ, g, μ . We have suppressed the ϕ -dependence. Initially, the activities $K_j = 0$, but they will arise under RG iterations and the form [49] remains stable, as we will see. The partition function density is thus parametrized as a couple (V, K) .

Norms for Polymer Activities

Polymer activities $K(X, \phi)$ are endowed with a norm $\|K(X)\|$, which must satisfy two properties:

$$\begin{aligned} \dot{X} \cap \dot{Y} = \emptyset &\Rightarrow \|K_1(X)K_2(Y)\| \leq \|K_1(X)\| \|K_2(Y)\| \\ \|T_L K(X)\| &\leq c^{|X|} \|K(X)\| \end{aligned} \quad [50]$$

where \dot{X} is the interior of X and $|X|$ is the number of blocks in X . c is a constant of order $O(1)$. The norm measures (Fréchet) differentiability properties of the activity $K(X, \phi)$ with respect to the field ϕ as well as its admissible growth in ϕ . The growth is admissible if it is μ_C integrable. The second property above ensures the stability of the norm under RG iteration. For a fixed polymer X , the norm is such that it gives rise to a Banach

space of activities $K(X)$. The final norm $\|\cdot\|_A$ incorporates the previous one and washes out the set dependence,

$$\|K\|_A = \sup_{\Delta} \sum_{X \supset \Delta} A(X) \|K(X)\| \quad [51]$$

where $A(X) = L^{(d+2)|X|}$. This norm essentially ensures that large polymers have small activities. The details of the above norms can be found in Brydges *et al.* (2003).

The RG operation map f is a composition of two maps. The RG iteration map $z \rightarrow T_L z$ induces a map $V \rightarrow \tilde{V}_L$ and a nonlinear map $\tilde{T}_L: K \rightarrow \tilde{K} = \tilde{T}_L(K)$. We then compose this with a (nonlinear) extraction map \mathcal{E} which takes out the expanding (relevant) parts of $\tilde{K} \rightarrow \mathcal{E}(\tilde{K}) = K'$ and compensates the local potential $\tilde{V}_L \rightarrow V'$ such that $T_L z$ remains invariant. We denote by f the composition of these two maps with

$$V \rightarrow V' = f_V(V, K), \quad K \rightarrow K' = f_K(V, K) \quad [52]$$

The Map \tilde{T}_L

Consider applying the RG map T_L to [49]. The map consists of a convolution $\mu_{\Gamma_L} *$ followed by the rescaling S_L . In the integration over the fluctuation field ζ , we will exploit the independence of $\zeta(x)$ and $\zeta(y)$ when $|x - y| \geq L$. To do this, we pave Λ by closed blocks of side L , called L -blocks, so that each L -block is a union of 1-blocks. Let \bar{X}^L be the L -closure of a set X , namely the smallest union of L -blocks containing X . The polymers will be combined into L -polymers which are, by definition, connected unions of L blocks. The combination is performed in such a way that the new polymers are associated to independent functionals of ζ .

Let $\tilde{V}(X, \phi)$, to be chosen later, be a local potential independent of ζ . For a coupling constant sufficiently small, there is a bound

$$\|e^{-V(Y)}\| \leq 2^{|Y|} \quad [53]$$

We assume that \tilde{V} is so chosen that the same bound holds when V is replaced by \tilde{V} . Define

$$P(\Delta, \zeta, \phi) = e^{-V(\Delta, \zeta + \phi)} - e^{-\tilde{V}(\Delta, \phi)} \quad [54]$$

Then we have

$$\begin{aligned} e^{-V(X_c, \zeta + \phi)} &= e^{-V(\bar{X}_c, \zeta + \phi)} \\ &= \prod_{\Delta \subset \bar{X}_c} (e^{-\tilde{V}(\Delta, \phi)} + P(\Delta, \zeta, \phi)) \end{aligned} \quad [55]$$

where \bar{X}_c is the closure of X_c . Expand out the product and insert into the representation [49] for

$z(\Lambda, \zeta + \phi)$. We then rewrite the resulting sum in terms of L -polymers. The sum splits into a sum over connected components. Define, for every connected L -polymer Y ,

$$\begin{aligned} BK(Y) &= \sum_{N+M \geq 1} \frac{1}{N!M!} \\ &\times \sum_{(X_j), (\Delta_i) \rightarrow Y} e^{-\tilde{V}(X_0)} \prod_{j=1}^N K(X_j) \prod_{i=1}^M P(\Delta_i) \end{aligned} \quad [56]$$

where $X_0 = Y \setminus (\cup X_j) \cup (\cup \Delta_i)$ and the sum over the distinct Δ_i , and disjoint 1-polymers X_j is such that their L -closure is Y . Equation [49] now becomes

$$z(\Lambda) = \sum \frac{1}{N!} \sum_{Y_1, \dots, Y_N} e^{-\tilde{V}(Y_c)} \prod_{j=1}^N BK(Y_j) \quad [57]$$

where the sum is over disjoint, connected closed L -polymers. We now perform the fluctuation integration over ζ followed by the rescaling. Now $\tilde{V}(Y_c)$ is independent of ζ . The ζ -integration sails through and then factorizes because the Y_j , being disjoint closed L -polymers, are separated from each other by a distance $\geq L$. The rescaling brings us back to 1-polymers and reduces the volume from Λ to $L^{-1}\Lambda$. Therefore,

$$\begin{aligned} z'(L^{-1}\Lambda) &= T_L z(\Lambda) \\ &= \sum \frac{1}{N!} \sum_{X_1, \dots, X_N} e^{-\tilde{V}_L(X_c)} \prod_{j=1}^N (T_L BK)(X_j) \end{aligned} \quad [58]$$

where the sum is over disjoint 1-polymers, $X_c = L^{-1}\Lambda \setminus X$. By definition $\tilde{V}_L(\Delta) = S_L \tilde{V}(L\Delta)$ and $(T_L BK)(Z) = S_L \mu_{\Gamma_L} * BK(LZ)$. This shows that the representation [49] is stable under iteration and, furthermore, gives us the map

$$\begin{aligned} V &\rightarrow \tilde{V}_L \\ K &\rightarrow \tilde{K} = \tilde{T}_L(K) = T_L BK \end{aligned} \quad [59]$$

The norm boundedness of K implies that $\tilde{T}_L(K)$ is norm bounded. We see from the above that a variation in the choice of \tilde{V} is reflected in the corresponding variation of \tilde{K} . The extraction map \mathcal{E} now takes out from \tilde{K} the expanding parts and then compensates it by a change of \tilde{V}_L in such a way that the representation [58] is left invariant by the simultaneous replacement $\tilde{V}_L \rightarrow V', \tilde{K} \rightarrow K' = \mathcal{E}(\tilde{K})$. The extraction map is nonlinear. Its linearization is a subtraction operation and this dominates in norm the nonlinearities, (Brydges *et al.* 1998).

The map $V \rightarrow \tilde{V}_L \rightarrow V'$ leads to a discrete flow of the coupling constants in V . It is convenient to write $K = K^{\text{pert}} + R$, where R is the remainder. Then the coupling constant flow is a discrete version of the

continuous flows encountered in the last section, together with remainders which are controlled by the size of R . In addition, we have the flow of K . The discrete flow of the pair (coupling constants, K) can be studied in a Banach space norm. Once one proves that the nonlinear parts satisfy a Lipschitz property, the discrete flow can be analyzed by the methods of stable-manifold theory of dynamical systems in a Banach space context. The reader is referred to the article by Brydges *et al.* (2003) for details of the extraction map and the application of stable-manifold theory in the construction of a global RG trajectory.

Further Topics

Lattice RG Methods

Statistical mechanical systems are often defined on a lattice. Moreover, the lattice provides an ultraviolet cutoff for Euclidean field theory compatible with Osterwalder–Schrader positivity. The standard lattice RG is based on Kadanoff–Wilson block spins. Its mathematical theory and applications have been developed by Balaban, and Gawedzki and Kupiainen (see Gawedzki and Kupiainen (1986) and references therein). This leads to multiscale decompositions of the Gaussian lattice field as a sum of independent fluctuation fields on increasing length scales. Brydges *et al.* (2004) have shown that standard Gaussian lattice fields have multiscale decompositions as a sum of independent fluctuation fields with the finite-range property introduced in the last section. This permits the development of rigorous lattice RG theory in the spirit of the continuum framework of the previous section.

Fermionic Field Theories

Field theories of interacting fermions are often simpler to handle than bosonic field theories. Because of statistics, fermion fields are bounded and perturbation series converges in finite volume in the presence of an ultraviolet cutoff. The notion of studying the RG flow at the level of effective potentials makes sense. At any given scale, there is always an ultraviolet cutoff and the fluctuation covariance being of fast decrease provides an infrared cutoff. This is illustrated by the work of Gawedzki and Kupiainen (1985), who gave a nonperturbative construction in the weak effective coupling regime of the RG trajectory for the Gross–Neveu model in two dimensions. This is an example of a model with an unstable Gaussian fixed point where the initial coupling has to be adjusted as a function of the

ultraviolet cutoff consistent with ultraviolet asymptotic freedom so as to stabilize the flow.

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See also: Operator Product Expansion in Quantum Field Theory; Renormalization: Statistical Mechanics and Condensed Matter.

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Falicov–Kimball Model

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A Brief History

The “Falicov–Kimball model” was first considered by Hubbard and Gutzwiller during 1963–65 as a simplification of the Hubbard model. In 1969, Falicov and Kimball introduced a model that included a few extra complications, in order to investigate metal–insulator phase transitions in rare-earth materials and transition-metal compounds (Falicov and Kimball 1969). Experimental data suggested that this transition is due to the interactions between electrons in two electronic states: nonlocalized states (itinerant electrons), and states that are localized around the sites corresponding to the metallic ions of the crystal (static electrons).

A tight-binding approximation leads to a model defined on a lattice (the crystal) and two species of particles are considered. The first species consists of spinless quantum fermions (we refer to them as “electrons”), and the second species consists of localized holes or electrons (“classical particles”). Electrons hop between nearest-neighbor sites but classical particles do not. Both species obey Fermi statistics (in particular, the Pauli exclusion principle prevents more than one particle of a given species to occupy the same site). Interactions are on-site and thus involve particles of different species; they can be repulsive or attractive.

The very simplicity of the model allows for a broad range of applications. It was studied in the context of mixed valence systems, binary alloys, and crystal formation. Adding a magnetic field yields the flux phase problem. The Falicov–Kimball model can also be viewed as the simplest model where quantum particles interact with classical fields.

The fifteen years following the introduction of the model saw studies based on approximate methods, such as Green’s function techniques, that gave rise to a lot of confusion. A breakthrough occurred in 1986 when Brandt and Schmidt, and Kennedy and Lieb, proposed the first rigorous results. In particular,

Kennedy and Lieb showed in their beautiful paper that the electrons create an effective interaction between the classical particles and that a phase transition takes place for any value of the coupling constant, provided the temperature is low enough.

Many studies by mathematical physicists followed and several results are presented in this short survey. Recent years have seen an increasing interest from condensed matter physicists. We encourage interested readers to consult the reviews by Freericks and Zlatić (2003), Gruber and Macris (1996), and Jędrzejewski and Lemáński (2001).

Mathematical Setting

Definitions

Let $\Lambda \subset \mathbb{Z}^d$ denote a finite cubic box. The configuration space for the classical particles is

$$\Omega_\Lambda = \{0, 1\}^\Lambda = \{\omega = (\omega_x) : x \in \Lambda, \text{ and } \omega_x = 0, 1\}$$

where $\omega_x = 0$ or 1 denotes the absence or presence of a classical particle at the site x . The total number of classical particles is $N_c(\omega) = \sum_{x \in \Lambda} \omega_x$. The Hilbert space for the spinless quantum particles (“electrons”) is the usual fermionic Fock space

$$\mathcal{F}_\Lambda = \bigoplus_{N=0}^{|\Lambda|} \mathcal{H}_{\Lambda, N}$$

where $\mathcal{H}_{\Lambda, N}$ is the Hilbert space of square summable, antisymmetric, complex functions $\Psi = \Psi(x_1, \dots, x_N)$ of N variables $x_i \in \Lambda$. Let a_x^\dagger and a_x denote the standard creation and annihilation operators of an electron at x ; recall that they satisfy the anticommutation relations

$$\{a_x, a_y\} = 0, \quad \{a_x^\dagger, a_y^\dagger\} = 0, \quad \{a_x, a_y^\dagger\} = \delta_{xy}$$

The Hamiltonian for the Falicov–Kimball model is an operator on \mathcal{F}_Λ that depends on the configurations of classical particles. Namely, for $\omega \in \Omega_\Lambda$, we define

$$H_\Lambda(\omega) = - \sum_{\substack{x, y \in \Lambda \\ |x-y|=1}} a_x^\dagger a_y - U \sum_{x \in \Lambda} \omega_x a_x^\dagger a_x$$

The first term represents the kinetic energy of the electrons. The second term represents the on-site attraction ($U > 0$) or repulsion ($U < 0$) between electrons and classical particles.

The Falicov–Kimball Hamiltonian can be written with the help of a one-body Hamiltonian h_Λ , which is an operator on the Hilbert space for a single electron $\ell^2(\Lambda)$. Indeed, we have

$$H_\Lambda(\omega) = \sum_{x,y \in \Lambda} h_{xy}(\omega) a_x^\dagger a_y$$

The matrix $h_\Lambda(\omega) = (h_{xy}(\omega))$ is the sum of a hopping matrix (adjacency matrix) t_Λ , and of a matrix $v_\Lambda(\omega)$ that represents an external potential due to the classical particles. Namely, we have

$$h_{xy}(\omega) = -t_{xy} - U\omega_x \delta_{xy}$$

where t_{xy} is one if x and y are nearest neighbors, and is zero otherwise. The spectrum of t_Λ lies in $(-2d, 2d)$, and the eigenvalues of $v_\Lambda(\omega)$ are $-U$ (with degeneracy $N_c(\omega)$) and 0 (with degeneracy $|\Lambda| - N_c(\omega)$). Denoting $\lambda_j(A)$ the eigenvalues of a matrix A , it follows from the minimax principle that

$$\lambda_j(A) - \|B\| \leq \lambda_j(A+B) \leq \lambda_j(A) + \|B\|$$

Let $\lambda_1(\omega) \leq \lambda_2(\omega) \leq \dots \leq \lambda_{|\Lambda|}(\omega)$ be the eigenvalues of $h_\Lambda(\omega)$. Choosing $A = v_\Lambda(\omega)$ and $B = t_\Lambda$ in the inequality above, we find that for $U > 0$,

$$\begin{aligned} -U - 2d &< \lambda_j(\omega) < -U + 2d \quad \text{for } j = 1, \dots, N_c(\omega) \\ -2d &< \lambda_j(\omega) < 2d \quad \text{for } j = N_c(\omega) + 1, \dots, |\Lambda| \end{aligned}$$

In particular, for any configuration ω and any Λ ,

$$\text{Spec } h_\Lambda(\omega) \subset (-U - 2d, -U + 2d) \cup (-2d, 2d)$$

Thus, for $U > 4d$, the spectrum of $h_\Lambda(\omega)$ has the “universal” gap $(-U + 2d, -2d)$. A similar property holds for $U < -4d$.

Canonical Ensemble

A fruitful approach towards understanding the behavior of the Falicov–Kimball model is to first fix the configuration of the classical particles, and then to introduce the ground-state energy $E_\Lambda(N_e, \omega)$ as the lowest eigenvalue of $H_\Lambda(\omega)$ in the subspace $\mathcal{H}_{\Lambda, N_e}$:

$$E_\Lambda(N_e, \omega) = \inf_{\Psi \in \mathcal{H}_{\Lambda, N_e}, \|\Psi\|=1} \langle \Psi | H_\Lambda(\omega) | \Psi \rangle = \sum_{j=1}^{N_e} \lambda_j(\omega)$$

A typical problem is to find the set of ground-state configurations, that is, the set of configurations that minimize $E_\Lambda(N_e, \omega)$ for given N_e and $N_c = N_c(\omega)$.

In the case $U > 4d$ and $N_e = N_c(\omega)$, the ground-state energy $E_\Lambda(N_c(\omega), \omega)$ has a convergent expansion in powers of U^{-1} :

$$\begin{aligned} E_\Lambda(N_c(\omega), \omega) &= -UN_c(\omega) + \sum_{k \geq 2} \frac{1}{kU^{k-1}} \\ &\times \sum_{\substack{x_1, \dots, x_k \in \Lambda \\ |x_i - x_{i-1}| = 1 \\ 0 < m(\{x_i\}) < k}} (-1)^{m(\{x_i\})} \binom{k-2}{m(\{x_i\})-1} \end{aligned} \quad [1]$$

where $m(x_1, \dots, x_k)$ is the number of sites x_i with $\omega_{x_i} = 0$. The last sum also includes the condition $|x_k - x_1| = 1$. Simple estimates show that the series is less than $(2d/(U - 4d))N_c(\omega)$. The lowest-order term is a nearest-neighbor interaction,

$$-\frac{1}{U} \sum_{\{x,y\}: |x-y|=1} \delta_{\omega_x, 1-\omega_y}$$

that favors pairs with different occupation numbers. Formula [1] is the starting point for most studies of the phase diagram for large U . A similar expansion holds for $U < -4d$ and $N_e = |\Lambda| - N_c(\omega)$.

A simple derivation of expansion [1] using Cauchy formula can be found in Gruber and Macris (1996). It can be extended to positive temperatures with the help of Lie–Schwinger series (Datta *et al.* 1999).

Phase diagrams are better discussed in the limit of infinite volumes where boundary effects can be discarded. Let Ω^{per} be the set of configurations on \mathbb{Z}^d that are periodic in all d directions, and $\Omega^{\text{per}}(\rho_c) \subset \Omega^{\text{per}}$ be the set of periodic configurations with density ρ_c . For $\omega \in \Omega^{\text{per}}$ and $\rho_e \in [0, 1]$, we introduce the energy per site in the infinite volume limit by

$$e(\rho_e, \omega) = \lim_{\Lambda \nearrow \mathbb{Z}^d} \frac{1}{|\Lambda|} E_\Lambda(N_e, \omega) \quad [2]$$

Here, the limit is taken over any sequence of increasing cubes, and $N_e = [\rho_e |\Lambda|]$ is the integer part of $\rho_e |\Lambda|$. Existence of this limit follows from standard arguments.

In the case of the empty configuration $\omega_x \equiv 0$, we get the well-known energy per site of free lattice electrons: for $k \in [-\pi, \pi]^d$, let $\varepsilon(k) = -\sum_{\nu=1}^d \cos k_\nu$; then

$$e(\rho_e, \omega \equiv 0) = \frac{1}{(2\pi)^d} \int_{\varepsilon(k) < \varepsilon_F(\rho_e)} \varepsilon(k) dk$$

where $\varepsilon_F(\rho_e)$ is the Fermi energy, defined by

$$\rho_e = \frac{1}{(2\pi)^d} \int_{\varepsilon(k) < \varepsilon_F(\rho_e)} dk$$

The other simple situation is the full configuration $\omega_x \equiv 1$, whose energy is $e(\rho_e, \omega \equiv 1) = e(\rho_e, \omega \equiv 0) - U\rho_e$.

Let $e(\rho_e, \rho_c)$ denote the absolute ground-state energy density, namely,

$$e(\rho_e, \rho_c) = \inf_{\omega \in \Omega^{\text{per}}(\rho_c)} e(\rho_e, \omega)$$

Notice that $e(\rho_e, \omega)$ is convex in ρ_e , and that $e(\rho_e, \rho_c)$ is the convex envelope of $\{e(\rho_e, \omega) : \omega \in \Omega^{\text{per}}(\rho_c)\}$. It may be locally linear around some (ρ_e, ρ_c) . This is the case if the infimum is not realized by a periodic configuration. The nonperiodic ground states can be expressed as linear combinations of two or more periodic ground states (“mixtures”). That is, for $1 \leq i \leq n$ there are $\alpha_i \geq 0$ with $\sum_i \alpha_i = 1$, $\omega^{(i)} \in \Omega^{\text{per}}$, and $\rho_e^{(i)}$, such that

$$\rho_e = \sum_i \alpha_i \rho_e^{(i)}, \quad \rho_c = \sum_i \alpha_i \rho_c(\omega^{(i)})$$

and

$$e(\rho_e, \rho_c) = \sum_i \alpha_i e(\rho_e^{(i)}, \omega^{(i)})$$

The simplest mixture is the “segregated state” for densities $\rho_e < \rho_c$: take $\omega^{(1)}$ to be the empty configuration, $\omega^{(2)}$ to be the full configuration, $\rho_e^{(1)} = 0$, $\rho_e^{(2)} = \rho_e/\rho_c$, and $\alpha_2 = 1 - \alpha_1 = \rho_c$.

If $d \geq 2$, a mixture between configurations $\omega^{(i)}$ can be realized as follows. First, partition \mathbb{Z}^d into domains $D_1 \cup \dots \cup D_n$ such that $|D_i|/|\Lambda| \rightarrow \alpha_i$ and $|\partial D_i|/|\Lambda| \rightarrow 0$ as $\Lambda \nearrow \mathbb{Z}^d$. Then, define a nonperiodic configuration ω by setting $\omega_x = \omega_x^{(i)}$ for $x \in D_i$ (see the illustration in Figure 1). The canonical energy can be computed from [2], and it is equal to

$$e(\rho_e, \omega) = \inf_{(\rho_e^{(i)}) : \sum_i \alpha_i \rho_e^{(i)} = \rho_e} \sum_{i=1}^n \alpha_i e(\rho_e^{(i)}, \omega^{(i)})$$

Furthermore, the infimum is realized by densities $\rho_e^{(i)}$ such that there exists μ_e with $\rho_e(\mu_e, \omega^{(i)}) = \rho_e^{(i)}$ for all i (see [4] below for the definition of $\rho_e(\mu_e, \omega)$).

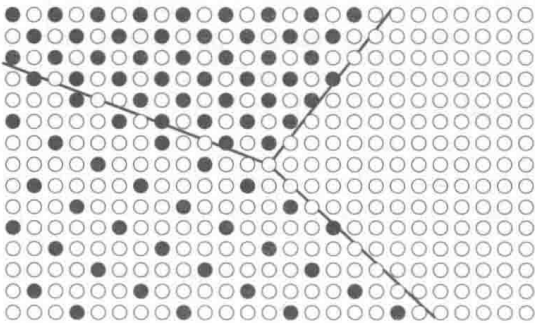


Figure 1 A two-dimensional mixed configuration formed by periodic configurations of densities 0, 1/5, and 1/2.

We define the *canonical ground-state phase diagram* as the set of ground states ω (either a periodic configuration or a mixture) that minimize the ground-state energy for given densities ρ_e, ρ_c :

$$G_{\text{can}}(\rho_e, \rho_c) = \{\omega : e(\rho_e, \omega) = e(\rho_e, \rho_c) \text{ and } \rho_c(\omega) = \rho_c\}$$

Grand-Canonical Ensemble

Properties of the system at finite temperatures are usually investigated within the grand-canonical formalism. The equilibrium state is characterized by an inverse temperature $\beta = 1/k_B T$, and by chemical potentials μ_e, μ_c , for the electrons and for the classical particles, respectively. In this formalism, the thermodynamic properties are derived from the partition functions

$$\begin{aligned} Z_\Lambda(\beta, \mu_e, \omega) &= \text{tr}_{\mathcal{F}_\Lambda} e^{-\beta[H_\Lambda(\omega) - \mu_e N_\Lambda]} \\ Z_\Lambda(\beta, \mu_e, \mu_c) &= \sum_{\omega \in \Omega_\Lambda} e^{\beta \mu_c N_c(\omega)} Z_\Lambda(\beta, \mu_e, \omega) \end{aligned} \quad [3]$$

Here, $N_\Lambda = \sum_{x \in \Lambda} a_x^\dagger a_x$ is the operator for the total number of electrons. We then define the free energy by

$$F_\Lambda(\beta, \mu_e, \mu_c) = -\frac{1}{\beta} \log Z_\Lambda(\beta, \mu_e, \mu_c)$$

The first partition function in [3] allows us to introduce an effective interaction for the classical particles, mediated by the electrons, by

$$F_\Lambda(\beta, \mu_e, \mu_c, \omega) = -\mu_c N_c(\omega) - \frac{1}{\beta} \log Z_\Lambda(\beta, \mu_e, \omega)$$

It depends on the inverse temperature β . Taking the limit of zero temperature gives the corresponding ground-state energy of the electrons in the classical configuration ω :

$$\begin{aligned} E_\Lambda(\mu_e, \mu_c, \omega) &= \lim_{\beta \rightarrow \infty} F_\Lambda(\beta, \mu_e, \mu_c, \omega) \\ &= -\mu_c N_c(\omega) + \sum_{j: \lambda_j(\omega) < \mu_e} (\lambda_j(\omega) - \mu_e) \end{aligned}$$

Notice that F_Λ and E_Λ are strictly decreasing and concave in μ_e, μ_c (E_Λ is actually linear in μ_c). We also define the energy density in the infinite volume limit by considering a sequence of increasing cubes. For $\omega \in \Omega^{\text{per}}$,

$$e(\mu_e, \mu_c, \omega) = \lim_{\Lambda \nearrow \mathbb{Z}^d} \frac{1}{|\Lambda|} E_\Lambda(\mu_e, \mu_c, \omega)$$

The corresponding electronic density is

$$\begin{aligned} \rho_e(\mu_e, \omega) &= \lim_{\Lambda \nearrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \# \{j : \lambda_j(\omega) < \mu_e\} \\ &= -\frac{\partial}{\partial \mu_e} e(\mu_e, \mu_c, \omega) \end{aligned} \quad [4]$$

and the density of classical particles is $\rho_c(\omega) = \lim_{\Lambda} N_c(\omega)/|\Lambda|$. One can check that canonical and grand-canonical energies are related by

$$e(\mu_e, \mu_c, \omega) = e(\rho_e(\mu_e, \omega), \omega) - \mu_e \rho_e(\mu_e, \omega) - \mu_c \rho_c(\omega) \quad [5]$$

Given (μ_e, μ_c) , the ground-state energy density $e(\mu_e, \mu_c)$ is defined by

$$e(\mu_e, \mu_c) = \inf_{\omega \in \Omega^{\text{per}}} e(\mu_e, \mu_c, \omega)$$

The set of periodic ground-state configurations for given chemical potentials μ_e, μ_c is the *grand-canonical ground-state phase diagram*:

$$G_{\text{gc}}(\mu_e, \mu_c) = \left\{ \omega \in \Omega^{\text{per}} : e(\mu_e, \mu_c, \omega) = e(\mu_e, \mu_c) \right\}$$

It may happen that no periodic configuration minimizes $e(\mu_e, \mu_c, \omega)$ and that $G_{\text{gc}}(\mu_e, \mu_c) = \emptyset$. However, results suggest that $G_{\text{gc}}(\mu_e, \mu_c)$ is nonempty for almost all μ_e, μ_c .

The situation simplifies for $U > 4d$ and $\mu_e \in (-U + 2d, -2d)$. Since μ_e belongs to the gap of $h_{\Lambda}(\omega)$, we have $\rho_e(\mu_e, \omega) = \rho_c(\omega)$, and

$$e(\mu_e, \mu_c, \omega) = e(\rho_c(\omega), \omega) - (\mu_e + \mu_c)\rho_c(\omega)$$

Thus, $G_{\text{gc}}(\mu_e, \mu_c)$ is invariant along the line $\mu_e + \mu_c = \text{const.}$ (for μ_e in the gap).

Symmetries of the Model

The Hamiltonian H_{Λ} clearly has the symmetries of the lattice (for a box with periodic boundary conditions, there is invariance under translations, rotations by 90° , and reflections through an axis). More important, it also possesses particle-hole symmetries and these are useful since they allow us to restrict investigations to positive U and to certain domains of densities or chemical potentials (see below).

- The classical particle-hole transformation $\omega_x \mapsto \bar{\omega}_x = 1 - \omega_x$ results in

$$H_{\Lambda}^U(\bar{\omega}) = H_{\Lambda}^{-U}(\omega) - UN_{\Lambda}$$

and $N_c(\bar{\omega}) = |\Lambda| - N_c(\omega)$. It follows that $E_{\Lambda}^U(N_e, \bar{\omega}) = E_{\Lambda}^{-U}(N_e, \omega) - UN_e$, and

$$G_{\text{can}}^{-U}(\rho_e, \rho_c) = \left\{ \bar{\omega} : \omega \in G_{\text{can}}^U(\rho_e, 1 - \rho_c) \right\}$$

$$G_{\text{gc}}^{-U}(\mu_e, \mu_c) = \left\{ \bar{\omega} : \omega \in G_{\text{gc}}^U(\mu_e - U, -\mu_c) \right\}$$

- An electron-hole transformation can be defined via the unitary transformation $a_x \mapsto \varepsilon_x a_x^\dagger$ and

$a_x^\dagger \mapsto \varepsilon_x a_x$, where $\varepsilon_x = 1$ on a sublattice, and $= -1$ on the other sublattice. Then,

$$H_{\Lambda}^U(\omega) \mapsto H_{\Lambda}^{-U}(\omega) - UN_c(\omega)$$

and $N_{\Lambda} \mapsto |\Lambda| - N_{\Lambda}$. It follows that $E_{\Lambda}^U(|\Lambda| - N_e, \omega) = E_{\Lambda}^{-U}(N_e, \omega) - UN_c(\omega)$, and

$$G_{\text{can}}^{-U}(\rho_e, \rho_c) = G_{\text{can}}^U(1 - \rho_e, \rho_c)$$

$$G_{\text{gc}}^{-U}(\mu_e, \mu_c) = G_{\text{gc}}^U(-\mu_e, \mu_c - U)$$

- Finally, the particle-hole transformation for both the classical particles and the electrons gives

$$H_{\Lambda}^U(\bar{\omega}) \mapsto H_{\Lambda}^U(\omega) + UN_{\Lambda} + UN_c(\omega) - U|\Lambda|$$

It follows that

$$E_{\Lambda}^U(|\Lambda| - N_e, \bar{\omega}) = E_{\Lambda}^U(N_e, \omega) + U(N_e + N_c(\omega) - |\Lambda|)$$

and

$$G_{\text{can}}^U(\rho_e, \rho_c) = \left\{ \bar{\omega} : \omega \in G_{\text{can}}^U(1 - \rho_e, 1 - \rho_c) \right\}$$

$$G_{\text{gc}}^U(\mu_e, \mu_c) = \left\{ \bar{\omega} : \omega \in G_{\text{gc}}^U(-\mu_e - U, -\mu_c - U) \right\}$$

Any of the first two symmetries allow us to choose the sign of U . We assume from now on that $U \geq 0$. The third symmetry indicates that the phase diagrams have a point of central symmetry, given by $\rho_e = \rho_c = 1/2$ in the canonical ensemble and $\mu_e = \mu_c = -U/2$ in the grand-canonical ensemble. Consequently, it is enough to study densities satisfying $\rho_e \leq 1/2$ and chemical potentials satisfying $\mu_e \leq -U/2$.

These symmetries also have useful consequences at positive temperatures. In particular, both species of particles have average density $1/2$ at $\mu_e = \mu_c = -U/2$, for all β .

The Ground State – Arbitrary Dimensions

The Segregated State

What follows is best understood in the limit $U \rightarrow \infty$ and when $\rho_e < \rho_c$. In this case, the electrons become localized in the domain $\mathcal{D}_{\Lambda}(\omega) = \{x \in \Lambda : \omega_x = 1\}$ and their energy per site is that of the full configuration, $e(\rho, \omega \equiv 1)$ (see the section “Canonical ensemble”), where $\rho = \rho_e/\rho_c$ is the effective electronic density. The presence of a boundary for $\mathcal{D}_{\Lambda}(\omega)$ raises the energy and the correction is roughly proportional to

$$B_{\Lambda}(\omega) = \# \left\{ (x, y) : x \in \mathcal{D}_{\Lambda}(\omega) \text{ and } y \in \mathbb{Z}^d \setminus \mathcal{D}_{\Lambda}(\omega) \right\}$$

The following theorem was proposed by Freericks *et al.* (2002).

Theorem 1

- (i) Let $\Lambda \subset \mathbb{Z}^d$ be a finite box, and $U > 4d$. Then for all $\omega \in \Omega_\Lambda$, and all $N_e \leq N_c(\omega) = N_c$, we have the following upper and lower bounds:

$$\frac{1}{2d} \left| e\left(\frac{N_e}{N_c}, \omega \equiv 0\right) \right| B_\Lambda(\omega) \geq E_\Lambda(N_e, \omega) - N_c e\left(\frac{N_e}{N_c}, \omega \equiv 1\right) \geq \left[a\left(\frac{N_e}{N_c}\right) - \gamma(U) \right] B_\Lambda(\omega)$$

Here, $a(\rho) = a(1 - \rho)$ is strictly positive for $0 < \rho < 1$. $\gamma(U)$ behaves as $8d^2/U$ for large U , in the sense that $U\gamma(U) \rightarrow 8d^2$ as $U \rightarrow \infty$.

- (ii) For any $\rho_e \neq \rho_c$ that differ from zero, the segregated state is the unique ground state if $a(\rho_e/\rho_c) > \gamma(U)$, that is, if U is large enough.

The proof of (i) is rather lengthy and we only show here that it implies (ii). Let $b(\omega) = \lim_\Lambda (B_\Lambda(\omega)/|\Lambda|)$, and notice that $b(\omega) = 0$ for the empty, the full, and the segregated configurations; $0 < b(\omega) < d$ for all other periodic configurations or mixtures. Recall that $\rho_c e(\rho_e/\rho_c, \omega \equiv 1)$ is the energy density of the segregated state. For all densities such that $a(\rho_e/\rho_c) > \gamma(U)$, and all configurations such that $\rho_c(\omega) = \rho_c$, we have

$$e(\rho_e, \omega) \geq \rho_c e\left(\frac{\rho_e}{\rho_c}, \omega \equiv 1\right)$$

and the inequality is strict for any periodic configuration. This shows that the segregated configuration is the unique ground state.

General Properties of the Grand-Canonical Phase Diagram

We have already seen that the grand-canonical phase diagram is symmetric with respect to $(-U/2, -U/2)$. Other properties follow from concavity of $e(\mu_e, \mu_c)$.

Let $\omega \in G_{gc}(\mu_e, \mu_c) \setminus G_{gc}(\mu'_e, \mu'_c)$ and $\omega' \in G_{gc}(\mu'_e, \mu'_c) \setminus G_{gc}(\mu_e, \mu_c)$. Then,

- (a) $\mu_e = \mu'_e$ and $\mu'_c > \mu_c$ imply $\rho_c(\omega') > \rho_c(\omega)$;
 (b) $\mu_c = \mu'_c$ and $\mu'_e > \mu_e$ imply $\rho_e(\mu'_e, \omega') > \rho_e(\mu_e, \omega)$, and ω cannot be obtained by adding some classical particles to the configuration ω' .

It follows from (b) that if $\omega \equiv 1 \in G_{gc}(\mu_e, \mu_c)$, then $\omega \equiv 1 \in G_{gc}(\mu'_e, \mu'_c)$ for all $\mu_e \geq \mu'_e, \mu_c \geq \mu'_c$. A similar property holds for the empty configuration. To establish these properties, we can start from

$$e(\mu_e, \mu_c, \omega') - e(\mu_e, \mu_c, \omega) > 0 > e(\mu'_e, \mu'_c, \omega') - e(\mu'_e, \mu'_c, \omega) \quad [6]$$

Since $e(\mu_e, \mu_c, \omega)$ is concave with respect to μ_e and linear with respect to μ_c , we have

$$e(\mu'_e, \mu'_c, \omega) \leq e(\mu_e, \mu_c, \omega) + (\mu_e - \mu'_e)\rho_e(\mu_e, \omega) + (\mu_c - \mu'_c)\rho_c(\omega) \quad [7]$$

Using this inequality for both terms on the right-hand side of [6], we obtain the inequality

$$(\mu'_e - \mu_e)[\rho_e(\mu'_e, \omega') - \rho_e(\mu_e, \omega)] + (\mu'_c - \mu_c)[\rho_c(\omega') - \rho_c(\omega)] \geq 0$$

which proves (a) and the first part of (b). The second part of (b) follows from

$$e(\mu_e, \mu_c, \omega) = - \int_{-\infty}^{\mu_e} d\mu \rho_e(\mu, \omega) - \mu_c \rho_c(\omega)$$

Indeed, the minimax principle implies that eigenvalues $\lambda_i(\omega)$ are decreasing with respect to ω (if $U \geq 0$), so that $\rho_e(\mu_e, \omega)$ is increasing (with respect to ω). Then for any $\omega'' > \omega$ and $\mu'_e > \mu_e$,

$$e(\mu'_e, \mu_c, \omega'') - e(\mu'_e, \mu_c, \omega) > e(\mu_e, \mu_c, \omega'') - e(\mu_e, \mu_c, \omega)$$

and $\omega'' \notin G_{gc}(\mu_e, \mu_c)$ implies $\omega'' \notin G_{gc}(\mu'_e, \mu'_c)$.

Next, we discuss domains in the plane of chemical potentials where the empty, full, and chessboard configurations have minimum energy (see, e.g., Gruber and Macris (1996), and references therein). One easily sees that $\omega \equiv 1$ is the unique ground-state configuration if $\mu_c > 0$, or if $\mu_e > 2d$ and $\mu_c > -U$. Similarly, $\omega \equiv 0$ is the unique ground state if $\mu_c < -U$, or if $\mu_e < -U - 2d$ and $\mu_c < 0$. For $U > 4d$, it follows from the expansion [1] that the full configuration is also ground state if $-U + 2d < \mu_e < -2d$ and $\mu_e + \mu_c + U > 4d/(U - 4d)$. These domains can be rigorously extended using energy estimates that involve correlation functions of classical particles. The results are illustrated in Figures 2 ($U < 4d$) and 3 ($U > 4d$).

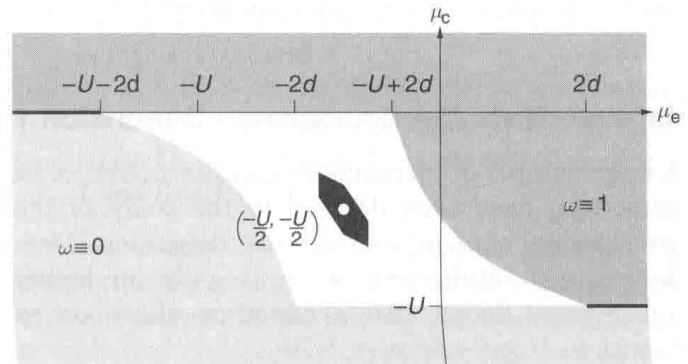


Figure 2 Grand-canonical ground-state phase diagram for $U < 4d$. Domains for the empty, chessboard, and full configurations, are denoted in light gray, black, and dark gray, respectively.

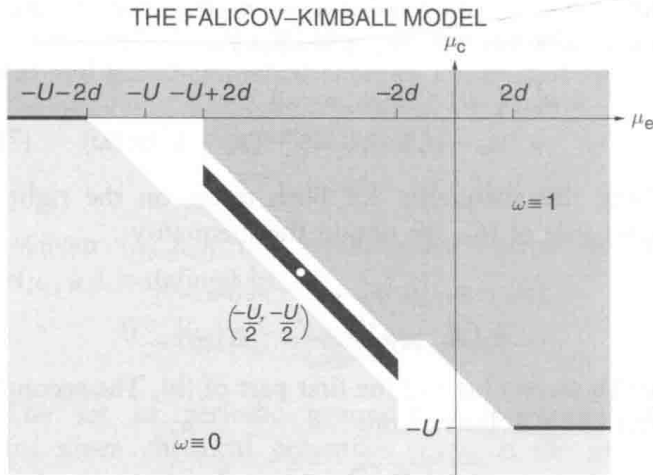


Figure 3 Grand-canonical ground-state phase diagram for $U > 4d$. Domains for the empty, chessboard, and full configurations are denoted in light gray, black, and dark gray, respectively.

Finally, canonical and grand-canonical phase diagrams are related by the following properties:

- (c) If $\omega \in G_{gc}(\mu_e, \mu_c)$, then $\omega \in G_{can}(\rho_e(\mu_e, \omega), \rho_c(\omega))$.
- (d) More generally, suppose that $\omega^{(1)}, \dots, \omega^{(n)} \in G_{gc}(\mu_e, \mu_c)$, and consider a mixture with coefficients $\alpha_1, \dots, \alpha_n$. The mixture belongs to $G_{can}(\rho_e, \rho_c)$, with $\rho_e = \sum_i \alpha_i \rho_e(\mu_e, \omega^{(i)})$ and $\rho_c = \sum_i \alpha_i \rho_c(\omega^{(i)})$.

To establish (c), observe that any ω' satisfies $e(\mu_e, \mu_c, \omega') \geq e(\mu_e, \mu_c, \omega)$ if $\omega \in G_{gc}(\mu_e, \mu_c)$. Let $\rho_e = \rho_e(\mu_e, \omega)$ and $\rho_c = \rho_c(\omega)$, and let μ'_e be such that $\rho_e(\mu'_e, \omega') = \rho_e$. By eqns [5] and [7],

$$\begin{aligned} e(\rho_e(\mu'_e, \omega'), \omega') - \mu_e \rho_e(\mu'_e, \omega') - \mu_c \rho_c(\omega') \\ \geq e(\rho_e(\mu_e, \omega), \omega) - \mu_e \rho_e(\mu_e, \omega) - \mu_c \rho_c(\omega) \end{aligned}$$

Then, $e(\rho_e, \omega') \geq e(\rho_e, \omega)$ for any configuration ω' such that $\rho_c(\omega') = \rho_c$. Property (d) follows from (c) by a limiting argument, because a mixture can be approximated by a sequence of periodic configurations.

Next we describe further properties of the phase diagrams that are specific to dimensions 1 and 2.

Ground-State Configurations – Dimension 1

A large number of investigations, either analytical or numerical, have been devoted to the study of the ground-state configurations in one dimension. One-dimensional results also serve as guide to higher dimensions. Recall that symmetries allow us to restrict to $U \geq 0$ and $\rho_e \leq 1/2$.

Most ground-state configurations that appear in the canonical phase diagram seem to be given by an intriguing formula, which we now describe. Let

$\rho_e = p/q$ with p relatively prime to q . Then corresponding periodic ground-state configurations have period q and density $\rho_c = r/q$ (r is an integer). The occupied sites in the cell $\{0, 1, \dots, q-1\}$ are given by the solutions k_0, \dots, k_{r-1} of

$$(pk_j) = j \bmod q, \quad 0 \leq j \leq r-1 \quad [8]$$

Note that the first classical particle is located at $k_0 = 0$, and k_0, \dots, k_{p-1} are *not* in increasing order. In order to discuss the solutions of [8], we introduce $\ell = [q/p]$ (the integer part of q/p), and we write

$$q = (\ell + 1)p - s \quad [9]$$

where $1 \leq s \leq p-1$, and s is relatively prime to p . Next, let $L(x)$ denote the distance between the particle at x and the one immediately preceding it (to the left).

Let us observe that if $\rho_c = \rho_e$, that is, if $r = p$, then

- (a) $L(k_j) = \ell$ for $0 \leq j \leq s-1$ and $k_j - \ell = k_{j+p-s}$.
- (b) $L(k_j) = \ell + 1$ for $s \leq j \leq p-1$ and $k_j - (\ell + 1) = k_{j-s}$.

Indeed, for $pk_j = j + nq$, eqn [9] implies

$$p(k_j - \ell) = j + (n-1)q + (p-s) = j + p - s \bmod q$$

and

$$p(k_j - \ell - 1) = j - s \bmod q$$

Therefore, $k_j - \ell$ is a solution of [8] if $j + p - s \leq p-1$, while $k_j - (\ell + 1)$ is a solution of [8] if $j - s \geq 0$.

These two properties show that the configuration defined by [8] is such that $L(x) \in \{\ell, \ell + 1\}$ for all occupied x . A periodic configuration such that all distances between consecutive particles are either ℓ or $\ell + 1$ is called *homogeneous*. Let ω be a homogeneous configuration with period q and density $\rho_c = r/q$, and let $x_0 < \dots < x_{p-1}$ be the occupied sites in $\{0, 1, \dots, q-1\}$. We introduce the *derivative* ω' of ω as the periodic configuration with period r defined by (see Figure 4)

$$\omega'_i = \begin{cases} 1 & \text{if } L(x_i) = \ell \\ 0 & \text{if } L(x_i) = \ell + 1 \end{cases}$$

A configuration is *most homogeneous* if it can be “differentiated” repeatedly until the empty or the full configuration is obtained.

Let ω be the homogeneous configuration from [8] and ω' be its derivative. Using the same arguments as for properties (a) and (b) above, and the fact that s is relatively prime to p , we obtain

- (c) Let k'_0, \dots, k'_{p-1} be the solutions of

$$(sk'_j) = j \bmod p$$

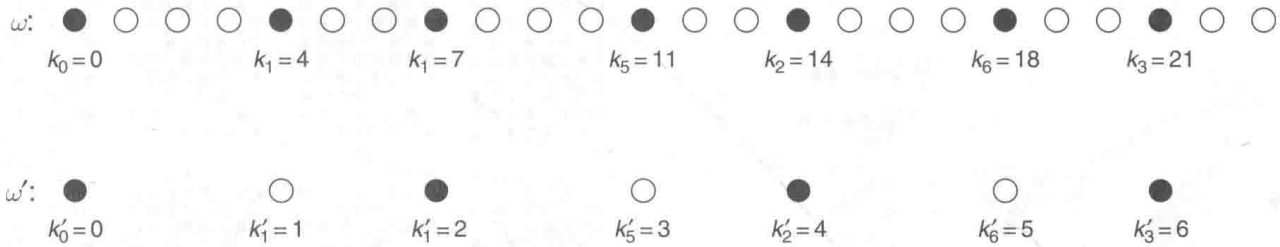


Figure 4 The configuration ω given by the formula [8] with $q=24$ and $p=7$, and its derivative ω' . Notice that $\ell=3$ and $s=4$.

Then (k'_0, \dots, k'_{p-1}) is a permutation of $(0, 1, \dots, p-1)$. Further, $k'_j - 1 = k'_{j+p-s}$ for $0 \leq j \leq s-1$, and $k'_j - 1 = k'_{j-s}$ for $s \leq j \leq p-1$.

Consider the periodic configuration with period p where sites k'_0, \dots, k'_{s-1} are occupied and sites k'_s, \dots, k'_{p-1} are empty. Since $k'_0=0$, this configuration is precisely the derivative ω' of ω . Iterating, these properties prove that the solutions of [8] are most homogeneous.

One of the most important results in one dimension is that only most homogeneous configurations are present in the canonical phase diagram, for U large enough and for equal densities $\rho_e = \rho_c$.

Theorem 2 Suppose that $\rho_e = \rho_c = p/q$. There exists a constant c such that for $U > c4^q$, the only ground-state configuration is the most homogeneous configuration, given by [8] (together with translations and reflections).

This theorem was established using the expansion [1] of $E_\Lambda(N_e, \omega)$ in powers of U^{-1} . It suggests a devil's staircase structure with infinitely many domains. However, the number of domains for fixed U could still be finite. Results from Theorem 2 are illustrated in Figure 5. Notice that $\rho_e = \rho_c$ when μ_e is in the universal gap. These results have been extended

to positive temperatures by using “quantum Pirogov–Sinai theory” (Datta *et al.* 1999).

For small U , on the other hand, one can use a (nonrigorous) Wigner–Brillouin degenerate perturbation theory (a standard tool in band theory). Let $\rho_e = p/q$ with p relatively prime to q , and ω be a periodic configuration with period $nq, n \in \mathbb{N}$. Then for U small enough ($U \ll 1/q$), we obtain the following expansion for the ground-state energy (Freericks *et al.* 1996):

$$e(\rho_e, \omega) = -\frac{2}{\pi} \sin \pi \rho_e - U \rho_e \rho_c(\omega) - \frac{|\hat{\omega}(\rho_e)|^2}{4\pi \sin \pi \rho_e} U^2 |\log U| + O(U^2) \quad [10]$$

where $\hat{\omega}(\rho_e)$ is the “structure factor” of the periodic configuration ω , namely

$$\hat{\omega}(\rho_e) = \frac{1}{nq} \sum_{j=0}^{nq-1} e^{-2\pi i \rho_e j} \omega_j$$

This expansion suggests that the ground-state configuration can be found by maximizing the structure factor. The following theorem holds independently of U .

Theorem 3 Let $\rho_e = p/q$. There exist $r_1 \geq q/4$ and $r_2 \leq 3q/4$ such that the configurations maximizing the structure factor are given as follows:

- (i) for $\rho_e = r/q$ with $r_1 \leq r \leq r_2$, use the formula [8];
- (ii) for $\rho_e \in (r/q, (r+1)/q)$ with $r_1 \leq r \leq r_2 - 1$, the configuration is a mixture of those for $\rho_e = r/q$ and $\rho_e = (r+1)/q$; and
- (iii) for $\rho_e \in (0, r_1/q)$, the configurations are mixtures of $\omega \equiv 0$ and that for $\rho_e = r_1/q$. For $\rho_e \in (r_2/q, 1)$, the configurations are mixtures of $\omega \equiv 1$ and that for $\rho_e = r_2/q$.

Some insight for low densities is provided by computing the energy of just one classical particle and one electron on the infinite line, and to compare it with two consecutive classical particles and two electrons. It turns out that the former is more favorable than the latter for $U > 2/\sqrt{3} \approx 1.15$, while “molecules” of two particles are forming

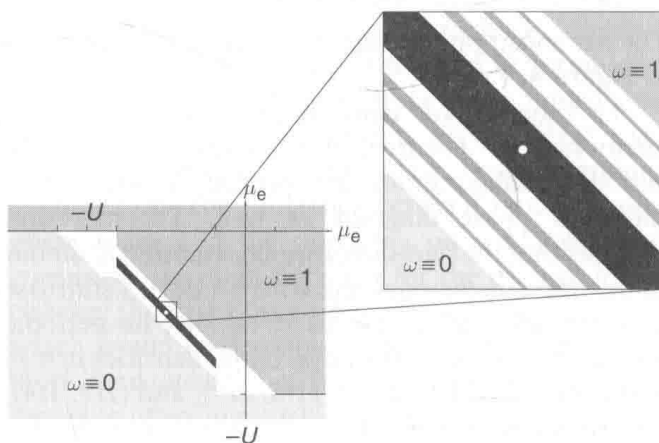


Figure 5 Grand-canonical ground-state phase diagram in one dimension for $U > 4$ and μ_e in the universal gap. Chessboard configurations occur in the black domain. Dark gray oblique domains correspond to densities $1/5, 1/4, 1/3, 2/3, 3/4, 4/5$. Total width of these domains is of order U^{-1} .

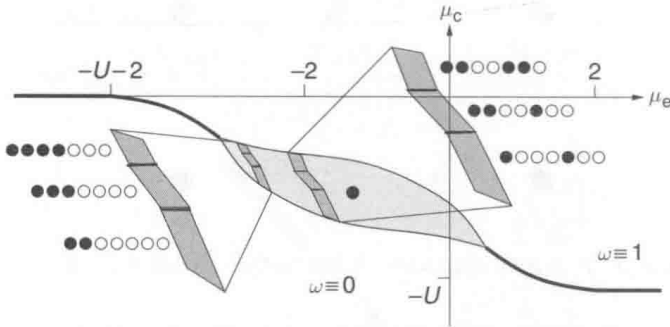


Figure 6 Grand-canonical ground-state phase diagram for $U \approx 0.4$. Enlarged are domains for $\rho_e = 1/7$ and $2/7$, with the same densities $\rho_c = 2/7, 3/7, 4/7$.

when $U < 2/\sqrt{3}$. Smaller U shows even bigger molecules for $\rho_c = n\rho_e$, and n -molecules are most homogeneously distributed according to the formula [8]. It should be stressed that the canonical ground state cannot be periodic if U is small and $\rho_c \notin [1/4, 3/4]$, which is different from the case of large U .

Only numerical results are available for intermediate U . They suggest that configurations occurring in the phase diagram are essentially given by Theorem 3 (together with the segregated configuration). This is sketched in Figure 6, where bold coexistence lines for $\mu_e > -U - 2$ and $\mu_e < 2$ represent segregated states.

Ground-State Configurations – Dimension 2

We discuss the canonical ensemble only, but many results extend to the grand-canonical ensemble. Recall that $G_{\text{can}}(1/2, 1/2)$ consists of the two chessboard configurations for any $U > 0$, and that segregation takes place when $\rho_e \neq \rho_c$, providing U is large enough (Theorem 1). Other results deal with the case of equal densities, and for U large enough (see Haller and Kennedy (2001), and references therein).

Theorem 4 Let $\rho_e = \rho_c \equiv \rho \leq 1/2$.

(i) If

$$\rho \in \left\{ \frac{1}{2}, \frac{2}{5}, \frac{1}{3}, \frac{1}{4}, \frac{2}{9}, \frac{1}{5}, \frac{2}{11}, \frac{1}{6} \right\}$$

then for U large enough, the ground-state configurations are those displayed in Figure 7. If $\rho = 1/(n^2 + (n+1)^2)$ with integer n , then for U large enough (depending on ρ), the ground-state configurations are periodic.

(ii) If ρ is a rational number between $1/3$ and $2/5$, then for U large enough (depending on the

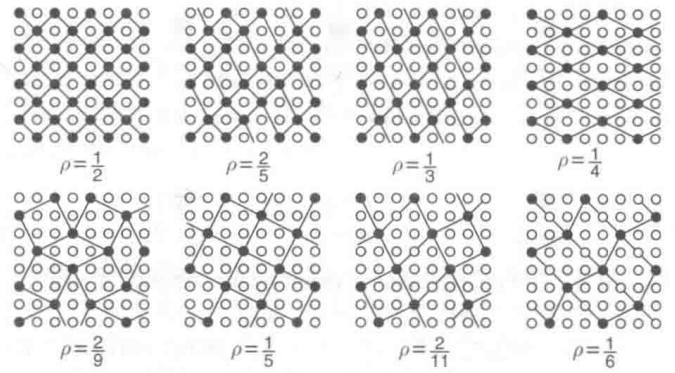


Figure 7 Ground-state configurations for several densities. Occupied sites are denoted by black circles, empty sites by white circles. Lines are present only to clarify the patterns.

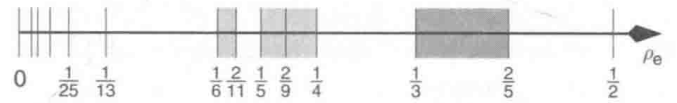


Figure 8 Canonical ground-state phase diagram in two dimensions for $U > 8$.

denominator of ρ), the ground-state configurations are periodic. Further, the restriction to any horizontal line is a one-dimensional periodic configuration given by [8], and the configuration is constant in either the direction $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ or $\begin{pmatrix} 1 \\ -1 \end{pmatrix}$.

(iii) Suppose that U is large enough. If $\rho \in (1/6, 2/11)$, the ground-state configurations are mixtures of the configurations $\rho = 1/6$ and $\rho = 2/11$ of Figure 7. If $\rho \in (1/5, 2/9)$, the ground-state configurations are mixtures of the configurations $\rho = 1/5$ and $\rho = 2/9$. If $\rho \in (2/9, 1/4)$, the ground-state configurations are mixtures of the configurations $\rho = 2/9$ and $\rho = 1/4$.

The canonical phase diagram for $\rho_e = \rho_c$ is presented in Figure 8.

The situation for densities $\rho \leq 1/2$ that are not mentioned in Theorem 4 is unknown. All these periodic configurations are present in the grand-canonical phase diagram as well. Theorem 4(ii) suggests that the two-dimensional situation is similar to the one-dimensional one where a devil's staircase structure may occur. Let us stress that no periodic configurations occur for large U and densities $\rho_e = \rho_c$ in the intervals $(1/6, 2/11)$, $(1/5, 2/9)$, and $(2/9, 1/4)$. This resembles the one-dimensional situation, but for small U .

See also: Quantum Spin Systems; Quantum Statistical Mechanics: Overview; Fermionic Systems; Hubbard Model; Pirogov–Sinai Theory.

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Fedosov Quantization

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Introduction

On the one hand, quantum mechanics and classical mechanics appear to be formulated within quite different mathematical frameworks, that is, in terms of Hilbert spaces and operators on Hilbert spaces on the quantum side and in terms of phase spaces, that is, symplectic, or more generally, Poisson manifolds, and functions on these phase spaces on the classical side. On the other hand, there is a strong structural similarity between the algebras of observable quantities in both theories which are associative \ast -algebras over \mathbb{C} . In the classical case, the algebra is commutative the product being the pointwise product of functions on the phase space and is endowed with the additional structure of a Poisson bracket by means of which the dynamics of the system can be formulated. In the quantum case, the algebra is the noncommutative composition of operators on a Hilbert space and the dynamics is determined by the corresponding commutator. The difference between functions on a phase space and the operators on a Hilbert space constitutes the main difficulty for the passage from a classical theory to the corresponding quantum theory which would be desirable, since a formulation of the more fundamental but much less intuitive quantum theory is often impossible. Even the consideration of the classical limit leads to the same problem of comparing quite different mathematical objects. One possibility, which is the basic idea of deformation quantization, to avoid these problems is to pass from classical observables to quantum observables not by

changing the underlying vector space, but only by deforming the algebraic structures namely the associative product and possibly the \ast -involution.

This idea motivates the following definition of a star product by Bayen *et al.* (1978), which reassembles the minimal demands made on a suitable quantization:

Definition 1 A star product on a Poisson manifold (M, Π) is an associative $\mathbb{C}[[\nu]]$ -bilinear product \star on $C^\infty(M)[[\nu]]$ such that – writing $f \star g = \sum_{r=0}^{\infty} \nu^r C_r(f, g)$ for $f, g \in C^\infty(M)$ with \mathbb{C} -bilinear maps C_r with values in $C^\infty(M)$ – the following properties hold:

- (i) $C_0(f, g) = fg$,
- (ii) $C_1(f, g) - C_1(g, f) = \{f, g\}$, and
- (iii) $1 \star f = f = f \star 1$.

In case the \mathbb{C} -bilinear maps C_r are differential operators, the star product is called differential. If $\bar{f} \star g = \bar{g} \star \bar{f}$, then \star is called Hermitian.

The conditions (i) and (ii) express the correspondence principle in deformation quantization and in case the star product converges the formal parameter is to be identified with $i\hbar$, whence we set $\bar{\nu} = -\nu$ considering the formal parameter as purely imaginary. Since the Fedosov star products we are going to study in the sequel are differential, we shall drop stressing this property explicitly and refer to differential star products as star products, merely.

One main advantage of deformation quantization is that one has the following very general existence result:

Theorem 1 On every Poisson manifold (M, Π) there exist (even differential) star products.

This theorem was first shown by DeWilde and Lecomte (1983) for the symplectic case and

independently by Fedosov (1985) who gave a beautiful explicit construction using geometrical structures on (M, ω) to build a star product recursively. Omori *et al.* (1991) gave yet another existence proof of star products on a symplectic manifold (M, ω) that appears to combine the methods of DeWilde and Lecomte (1983) and Fedosov (1985). The general proof of existence on general Poisson manifolds is due to Kontsevich (2003) and is a consequence of Kontsevich's formality theorem.

If $S = \text{id} + \sum_{r=1}^{\infty} \nu^r S_r$ is a formal series of differential operators on $C^\infty(M)$ with $S_r 1 = 0$ for $r \geq 1$, then

$$f \star' g := S^{-1}((Sf) \star (Sg)) \quad [1]$$

again defines a star product. Clearly, \star' is Hermitian in case \star is Hermitian and $S\bar{f} = \bar{Sf}$ for all $f \in C^\infty(M)[[\nu]]$. The above observation of the shape of certain isomorphisms between star product algebras gives rise to the notion of equivalence of star products:

Definition 2 Two star products \star and \star' on (M, Π) are called equivalent in case there is a formal series $S = \text{id} + \sum_{r=1}^{\infty} \nu^r S_r$ of differential operators on $C^\infty(M)$ with $S_r 1 = 0$ for $r \geq 1$ such that eqn [1] is satisfied for all $f, g \in C^\infty(M)[[\nu]]$.

The full classification of star products up to equivalence was first obtained in the symplectic case by Nest and Tsygan (1995) and independently by Deligne (1995) and Bertelson *et al.* (1997). The general Poisson case again follows from Kontsevich's formality theorem. In particular, in the symplectic case, star products are classified in a functorial way by the characteristic class

$$c : \star \mapsto c(\star) \in \frac{[\omega]}{\nu} + H_{\text{deRham}}^2(M)[[\nu]] \quad [2]$$

defined by Deligne that induces a bijection between the equivalence classes of star products and $[\omega]/\nu + H_{\text{deRham}}^2(M)[[\nu]]$. Moreover, it has been shown (Bertelson *et al.* 1997, Deligne 1995, Nest and Tsygan 1995) that every star product on a symplectic manifold is equivalent to a Fedosov star product. This fact can also be seen as a direct consequence of the explicit computation of the characteristic class of a Fedosov star product (cf. Neumaier (2002)). The importance of Fedosov's construction for the general theory of deformation quantization in the symplectic case is also shown by the fact that in many proofs Fedosov's star products were used to have reference star products to compare with a given star product. Moreover,

there is a great variety of modifications and generalizations of Fedosov's method and there are many examples where additional structures on the symplectic manifold suggest to look for star products adapted to them, where modified Fedosov constructions can be applied successfully.

Fedosov Star Products on (M, ω)

The attempt to construct a star product step by step in fact leads to a cohomological problem, where *a priori* an obstruction in the third Hochschild cohomology of $C^\infty(M)$ occurs. This problem results from the demand for associativity which is the really most restricting condition on a star product. Therefore, additional arguments are necessary to show that these obstructions can be circumvented, since the concerning cohomology is isomorphic to $\Gamma^\infty(\wedge^3 TM)$ and hence, for $\dim(M) \geq 3$, is not trivial at all.

The basic strategy of Fedosov's construction to build in associativity of the resulting product is to begin with a "very large" associative algebra $(\mathcal{W} \otimes \Lambda, \circ)$, where \circ mimicks the well-known Weyl–Moyal star product on a vector space with a constant symplectic Poisson tensor, and to specify a suitable subalgebra which is in bijection to $C^\infty(M)[[\nu]]$. Pulling back the product to the subalgebra then clearly results in an associative product on $C^\infty(M)[[\nu]]$, but as we shall see later on, one has to care for the bijection to be sufficiently nontrivial in order to obtain in fact a nontrivial deformation of the usual pointwise product on $C^\infty(M)[[\nu]]$.

Defining

$$\mathcal{W} \otimes \Lambda := \left(\bigtimes_{s=0}^{\infty} \Gamma^\infty(\bigvee^s T^*M \otimes \wedge^s T^*M) \right)[[\nu]] \quad [3]$$

$\mathcal{W} \otimes \Lambda$ becomes in a natural way an associative, supercommutative algebra using the symmetric \vee -product in the first factor and the antisymmetric \wedge -product in the second factor. This product is denoted by $\mu(a \otimes b) = ab$ for $a, b \in \mathcal{W} \otimes \Lambda$. By $\mathcal{W} \otimes \Lambda^k$ we denote the elements of antisymmetric degree k and set $\mathcal{W} := \mathcal{W} \otimes \Lambda^0$. Besides this pointwise product, the Poisson tensor Π corresponding to ω gives rise to another associative product \circ on $\mathcal{W} \otimes \Lambda$ by

$$a \circ b = \mu \left(\exp \left(\frac{\nu}{2} \Pi^j i_s(\partial_i) \otimes i_s(\partial_j) \right) (a \otimes b) \right) \quad [4]$$

which is a deformation of μ . Here $i_s(Y)$ denotes the symmetric insertion of a vector field $Y \in \Gamma^\infty(TM)$ and similarly $i_a(Y)$ shall be used to denote the antisymmetric insertion of a vector field. We set $\text{ad}(a)b := [a, b]$, where the latter denotes the

\deg_a -graded supercommutator with respect to \circ . Denoting the obvious degree maps by \deg_s, \deg_a , and $\deg_\nu = \nu \partial_\nu$, one observes that they all are derivations with respect to μ but \deg_s and \deg_ν fail to be derivations with respect to \circ . Instead, $\text{Deg} := \deg_s + 2\deg_\nu$ is a derivation of \circ and hence $(\mathcal{W} \otimes \Lambda, \circ)$ is formally Deg-graded and the corresponding degree is referred to as the total degree. Sometimes we write $\mathcal{W}_k \otimes \Lambda$ to denote the elements of total degree $\geq k$. The total degree can be used to define an ultrametric d on $\mathcal{W} \otimes \Lambda$ and it is known that $(\mathcal{W} \otimes \Lambda, d)$ is complete, which implies that Banach's fixed-point theorem can be applied in this setting. This observation is important since all the proofs of existence and uniqueness of certain elements in $\mathcal{W} \otimes \Lambda$ we shall construct in the sequel can be reduced to the application of this theorem.

In local coordinates, we define the differential

$$\delta := (1 \otimes dx^i) i_s(\partial_i) \quad [5]$$

which satisfies $\delta^2 = 0$ and is a superderivation of \circ . Evaluated at a point $m \in M$, the product $a(m)b(m)$ of two elements $a, b \in \mathcal{W} \otimes \Lambda$ can be considered as the \wedge -product of two differential forms with polynomial coefficient functions on the vector space $T_m M$. Interpreted this way, the restriction of δ to the fiber at m is nothing but the exterior derivative of differential forms with polynomial coefficients. Hence, it is clear that there is a homotopy operator δ^{-1} satisfying

$$\delta \delta^{-1} + \delta^{-1} \delta + \sigma = \text{id} \quad [6]$$

where $\sigma: \mathcal{W} \otimes \Lambda \rightarrow C^\infty(M)[[\nu]]$ denotes the projection onto the part of symmetric and antisymmetric degree 0. With the above view of δ , this is just the Poincaré Lemma for differential forms with polynomial coefficients, which says that all the cohomology spaces vanish except for the one of degree 0 and the cohomology in degree 0 is just given by the constant functions on the vector space $T_m M$. This means that the δ -cohomology on $\mathcal{W} \otimes \Lambda$ is trivial except for the space of degree 0, which is given by the formal functions on M . For computational purposes, it is useful to have a concrete formula of the homotopy operator δ^{-1} which is given by

$$\delta^{-1} a := \begin{cases} \frac{1}{k+l} (dx^i \otimes 1) i_a(\partial_i) a & \text{for } \deg_s a = ka, \\ \deg_a a = la \text{ with } k+l \neq 0 & \\ 0 & \text{else} \end{cases} \quad [7]$$

Now $\ker(\delta) \cap \mathcal{W} = C^\infty(M)[[\nu]]$ and one might wonder whether this subalgebra of $(\mathcal{W} \otimes \Lambda, \circ)$ is already suitable to induce a deformed product on $C^\infty(M)[[\nu]]$ by pulling back the product \circ from $\mathcal{W} \otimes \Lambda$.

Evidently, the answer to the question is negative since the resulting product just gives back the undeformed pointwise product of formal functions on M . Hence one has to find a less trivial superderivation of the product \circ the kernel of which is still in bijection to $C^\infty(M)[[\nu]]$. The essential new component of Fedosov's construction is a superderivation of $(\mathcal{W} \otimes \Lambda, \circ)$ that is not $C^\infty(M)[[\nu]]$ -linear and hence in a certain sense generates derivatives along the base manifold M . Using a torsion-free symplectic connection ∇ on M we define an endomorphism also denoted by ∇ of $\mathcal{W} \otimes \Lambda$ by

$$\nabla := (1 \otimes dx^i) \nabla_{\partial_i} \quad [8]$$

which turns out to be a superderivation of \circ due to the fact that $\nabla \omega = \nabla \Pi = 0$. The map ∇ satisfies the identities

$$[\delta, \nabla] = 0, \quad \text{since the connection is torsion-free} \quad [9]$$

$$\nabla^2 = -\frac{1}{\nu} \text{ad}(R),$$

$$\text{where } R := \frac{1}{4} \omega_{it} R_{jkl}^t dx^i \vee dx^j \otimes dx^k \wedge dx^l \in \mathcal{W} \otimes \Lambda^2 \quad [10]$$

involves the curvature of the connection. Moreover, we have

$$\delta R = 0 = \nabla R \quad [11]$$

by the Bianchi identities.

Now one could consider the superderivation $-\delta + \nabla$ of $(\mathcal{W} \otimes \Lambda, \circ)$ and try to define a mapping τ from $C^\infty(M)[[\nu]]$ to $\ker(-\delta + \nabla) \cap \mathcal{W}$ such that $\sigma(\tau(f)) = f$ for all $f \in C^\infty(M)[[\nu]]$. But in case the curvature of the connection does not vanish, the necessary condition for the solvability of the equation $(-\delta + \nabla)\tau(f) = 0$ subject to the additional condition $\sigma(\tau(f)) = f$ is not satisfied. Only in case there is a torsion-free symplectic connection on M with vanishing curvature, this procedure can be carried through and yields again the Weyl–Moyal star product since the fact that ∇ is symplectic in this case implies that the components of the Poisson tensor are constant. However, in general, the kernel of $-\delta + \nabla$ does not have the desired properties to specify a suitable subalgebra of $(\mathcal{W} \otimes \Lambda, \circ)$ and one makes the ansatz

$$\mathfrak{D} = -\delta + \nabla - \frac{1}{\nu} \text{ad}(r) \quad [12]$$

with an element $r \in \mathcal{W}_3 \otimes \Lambda^1$ for a suitable superderivation. Now a direct computation yields that

$$\mathfrak{D}^2 = \frac{1}{\nu} \text{ad} \left(\delta r - \nabla r + \frac{1}{\nu} r \circ r - R \right) \quad [13]$$

which vanishes iff $\delta r - \nabla r + (1/\nu)r \circ r - R$ is a central element in $\mathcal{W}_2 \otimes \Lambda^2$. This is the case iff there is a formal series of 2-forms $\Omega \in \nu\Gamma^\infty(\wedge^2 T^*M)[[\nu]]$ with

$$\delta r - \nabla r + \frac{1}{\nu}r \circ r - R = 1 \otimes \Omega \quad [14]$$

After these preparations, one is in the position to prove the following theorem:

Theorem 2 (Fedosov 1994, theorem 3.2; Fedosov 1996, theorem 5.2.2). *For every formal series $\Omega \in \nu\Gamma^\infty(\wedge^2 T^*M)[[\nu]]$ of closed 2-forms there exists a unique element $r \in \mathcal{W}_3 \otimes \Lambda^1$ such that*

$$\delta r = \nabla r - \frac{1}{\nu}r \circ r + R + 1 \otimes \Omega \quad \text{and} \quad \delta^{-1}r = 0 \quad [15]$$

Moreover, r satisfies

$$r = \delta^{-1} \left(R + 1 \otimes \Omega + \nabla r - \frac{1}{\nu}r \circ r \right) \quad [16]$$

from which r can be determined recursively. In this case the Fedosov derivation

$$\mathfrak{D} := -\delta + \nabla - \frac{1}{\nu}\text{ad}(r) \quad [17]$$

is a superderivation of antisymmetric degree 1 and has square zero: $\mathfrak{D}^2 = 0$.

For obvious reasons Fedosov calls \mathfrak{D} a flat or abelian connection for the bundle $\mathcal{W} \otimes \Lambda$ and $\omega + \Omega$ is referred to as the central Weyl curvature of the connection \mathfrak{D} . In some sense, the flatness property $\mathfrak{D}^2 = 0$ guarantees that there are sufficiently many flat sections. Before investigating the structure of $\ker(\mathfrak{D}) \cap \mathcal{W}$ we note that the \mathfrak{D} -cohomology is trivial on elements a with positive antisymmetric degree since one has the following homotopy formula:

$$\mathfrak{D}\mathfrak{D}^{-1}a + \mathfrak{D}^{-1}\mathfrak{D}a = a$$

where

$$\mathfrak{D}^{-1}a := -\delta^{-1} \left(\frac{1}{\text{id} - [\delta^{-1}, \nabla - (1/\nu)\text{ad}(r)]} a \right) \quad [18]$$

(cf. Fedosov (1996, theorem 5.2.5)). The reason for this fact, which is also the crucial point for the proof of Theorem 1, is the property of the δ -cohomology to vanish except for the cohomology space of degree 0.

The next step in Fedosov's construction now consists in establishing a bijection between the flat sections $a \in \mathcal{W}$, that is, those elements of \mathcal{W} with $\mathfrak{D}a = 0$, and $C^\infty(M)[[\nu]]$.

Theorem 3 (Fedosov 1994, theorem 3.3, Fedosov 1996, theorem 5.2.4). *Let $\mathfrak{D} = -\delta + \nabla - (1/\nu)$*

ad(r): $\mathcal{W} \otimes \Lambda \rightarrow \mathcal{W} \otimes \Lambda$ be given as in [17] with r as in [15].

- (i) *Then for any $f \in C^\infty(M)[[\nu]]$ there exists a unique element $\tau(f) \in \ker(\mathfrak{D}) \cap \mathcal{W}$ such that*

$$\sigma(\tau(f)) = f \quad [19]$$

and $\tau: C^\infty(M)[[\nu]] \rightarrow \ker(\mathfrak{D}) \cap \mathcal{W}$ is $C[[\nu]]$ -linear and referred to as the Fedosov–Taylor series corresponding to \mathfrak{D} .

- (ii) *In addition, $\tau(f)$ can be obtained recursively for $f \in C^\infty(M)$ from*

$$\tau(f) = f + \delta^{-1} \left(\nabla \tau(f) - \frac{1}{\nu}\text{ad}(r)\tau(f) \right) \quad [20]$$

Using \mathfrak{D}^{-1} according to [18] one can also write

$$\tau(f) = f - \mathfrak{D}^{-1}(1 \otimes \text{d}f) \quad \text{for all } f \in C^\infty(M)[[\nu]] \quad [21]$$

- (iii) *Since \mathfrak{D} as constructed above is a \circ -superderivation, $\ker(\mathfrak{D}) \cap \mathcal{W}$ is a \circ -subalgebra and a new associative product $*$ for $C^\infty(M)[[\nu]]$, which turns out to be a star product, is defined by pullback of \circ via τ :*

$$f * g := \sigma(\tau(f) \circ \tau(g)) \quad [22]$$

In the following, we shall refer to the associative product $*$ defined above as the Fedosov star product corresponding to (∇, Ω) . The choice of the formal series of closed 2-forms Ω in fact has a crucial effect on the equivalence class of the resulting star product, whereas the choice of the torsion-free symplectic connection, which in contrast to a Riemannian connection is not unique, does not affect this class. This observation has been the main step in all the proofs of the classification results in deformation quantization of symplectic manifolds. Another way to prove this fact is to compute the characteristic class $c(*)$ introduced by Deligne (1995) using the methods developed in Gutt and Rawnsley (1999) directly which yields:

Theorem 4 (Neumaier 2002, theorem 2). *Deligne's characteristic class $c(*)$ of a Fedosov star product $*$ as constructed above is given by*

$$c(*) = \frac{1}{\nu}[\omega] + \frac{1}{\nu}[\Omega] \quad [23]$$

The properties of Ω with respect to complex conjugation also decide on whether $*$ is Hermitian or not. In case Ω is real, that is, satisfies $\bar{\Omega} = \Omega$ it is easy to show – observing that $\bar{a} \circ b = (-1)^{kl} \bar{b} \circ a$ for $a \in \mathcal{W} \otimes \Lambda^k, b \in \mathcal{W} \otimes \Lambda^l$ – that \bar{r} solves the equations that uniquely determine r and hence $\bar{r} = r$. But then \mathfrak{D} commutes with complex conjugation and

therefore the unique characterization of the Fedosov–Taylor series yields $\tau(\bar{f}) = \tau(f)$ for all $f \in C^\infty(M)[[\nu]]$, implying that $*$ is Hermitian.

Derivations, Automorphisms, and Equivalence Transformations

Having defined the Fedosov star product $*$ corresponding to (∇, Ω) , the next logical step is to investigate the structure of its derivations and automorphisms and to find out how they can be described in the framework of Fedosov’s construction. In addition, one can ask for an explicit construction of equivalence transformations between two Fedosov star products $*$ and $*$ ' obtained from (∇, Ω) and (∇', Ω') that exist according to Theorem 4 iff $[\Omega] = [\Omega']$.

Since the basic philosophy of Fedosov’s construction is to consider suitable operations on the algebra $(\mathcal{W} \otimes \Lambda, \circ)$ in order to obtain induced mappings on the level of $(C^\infty(M)[[\nu]], *)$, one may expect to be able to define derivations of $(C^\infty(M)[[\nu]], *)$ by considering appropriate fiberwise quasi-inner derivations of $(\mathcal{W} \otimes \Lambda, \circ)$ of the shape

$$\mathcal{D}_h = -\frac{1}{\nu} \text{ad}(h) \quad [24]$$

where $h \in \mathcal{W}$ and without loss of generality we assume $\sigma(h) = 0$. Our aim is to define $\mathbb{C}[[\nu]]$ -linear derivations of $*$ by $C^\infty(M)[[\nu]] \ni f \mapsto \sigma(\mathcal{D}_h \tau(f))$, but for an arbitrary element $h \in \mathcal{W}$ with $\sigma(h) = 0$ this mapping fails to be a derivation as \mathcal{D}_h does not map elements of $\ker(\mathfrak{D}) \cap \mathcal{W}$ to elements of $\ker(\mathfrak{D}) \cap \mathcal{W}$. In order to achieve this, the supercommutator of \mathfrak{D} and \mathcal{D}_h has to vanish. As \mathfrak{D} is a $\mathbb{C}[[\nu]]$ -linear \circ -superderivation, we obviously have

$$[\mathfrak{D}, \mathcal{D}_h] = -\frac{1}{\nu} \text{ad}(\mathfrak{D}h) \quad [25]$$

and hence obviously $\mathfrak{D}h$ must be central, that is, $\mathfrak{D}h$ has to be of the shape $1 \otimes B$ with $B \in \Gamma^\infty(T^*M)[[\nu]]$ to have $[\mathfrak{D}, \mathcal{D}_h] = 0$. From $\mathfrak{D}^2 = 0$, we get that the necessary condition for the solvability of the equation $\mathfrak{D}h = 1 \otimes B$ is the closedness of B since $\mathfrak{D}(1 \otimes B) = 1 \otimes dB$. But as the \mathfrak{D} -cohomology is trivial on elements with positive antisymmetric degree, this condition is also sufficient for the solvability of the equation $\mathfrak{D}h = 1 \otimes B$ and we get the following statement.

Lemma 1 (Müller-Bahns and Neumaier 2004, lemma 2.1).

- (i) For all formal series $B \in \Gamma^\infty(T^*M)[[\nu]]$ of closed 1-forms on M there is a uniquely determined element $h_B \in \mathcal{W}$ such that $\mathfrak{D}h_B = 1 \otimes B$ and $\sigma(h_B) = 0$. Moreover, h_B is explicitly given by

$$h_B = \mathfrak{D}^{-1}(1 \otimes B) \quad [26]$$

- (ii) For all $B \in Z_{\text{deRham}}^1(M)[[\nu]]$ the mapping $D_B : C^\infty(M)[[\nu]] \rightarrow C^\infty(M)[[\nu]]$, where

$$D_B f := \sigma(\mathcal{D}_{h_B} \tau(f)) = \sigma\left(-\frac{1}{\nu} \text{ad}(h_B) \tau(f)\right) \quad [27]$$

for $f \in C^\infty(M)[[\nu]]$ defines a $\mathbb{C}[[\nu]]$ -linear derivation of $*$ and hence this construction yields a mapping $Z_{\text{deRham}}^1(M)[[\nu]] \ni B \mapsto D_B \in \text{Der}_{\mathbb{C}[[\nu]]}(C^\infty(M)[[\nu]], *)$.

Furthermore, one can show that one even obtains all $\mathbb{C}[[\nu]]$ -linear derivations of $*$ by varying B in the derivations D_B constructed above.

Proposition 1 (Müller-Bahns and Neumaier 2004, proposition 2.2). The mapping

$$Z_{\text{deRham}}^1(M)[[\nu]] \ni B \mapsto D_B \in \text{Der}_{\mathbb{C}[[\nu]]}(C^\infty(M)[[\nu]], *)$$

defined in Lemma 1 is a bijection. Moreover, D_{df} is a quasi-inner derivation for all $f \in C^\infty(M)[[\nu]]$, that is, $D_{df} = (1/\nu) \text{ad}_*(f)$ and the induced mapping $[B] \mapsto [D_B]$ from $H_{\text{deRham}}^1(M)[[\nu]]$ to $\text{Der}_{\mathbb{C}[[\nu]]}(C^\infty(M)[[\nu]], *) / \text{Der}_{\mathbb{C}[[\nu]]}^{\text{qi}}(C^\infty(M)[[\nu]], *)$ the space of $\mathbb{C}[[\nu]]$ -linear derivations of $*$ modulo the quasi-inner derivations, also is bijective.

Actually, it is well known that for an arbitrary star product $*$ on a symplectic manifold the space of $\mathbb{C}[[\nu]]$ -linear derivations is in bijection with $Z_{\text{deRham}}^1(M)[[\nu]]$ and that the quotient space of these derivations modulo the quasi-inner derivations is in bijection with $H_{\text{deRham}}^1(M)[[\nu]]$ (cf. Bertelson *et al.* (1997), theorem 4.2), but the remarkable thing about Fedosov star products is that these bijections can be explicitly expressed in terms of \mathfrak{D} resp. \mathfrak{D}^{-1} in a very lucid way.

Now we turn to the consideration of $\mathbb{C}[[\nu]]$ -linear automorphisms of $*$. For such automorphisms that start with id , which are also called self-equivalences, it is known (cf. Gutt and Rawnsley (1999), Proposition 3.3) for arbitrary star products $*$ on (M, ω) that they are of the form

$$A = \exp(\nu D) \quad [28]$$

with a $\mathbb{C}[[\nu]]$ -linear derivation D of $*$. Therefore, the above result about the description of all the derivations of $*$ directly yields a complete description of all self-equivalences of $*$.

The description of $\mathbb{C}[[\nu]]$ -linear automorphisms that are not self-equivalences of $*$ is slightly more involved and we first need some results about the concrete structure of the equivalence transformations between two Fedosov star products $*$ and $*$ '. To compare two Fedosov star products obtained from different torsion-free symplectic connections

∇ and ∇' and different but cohomologous formal series of 2-forms Ω and Ω' , one has to compare the corresponding Fedosov derivations \mathfrak{D} and \mathfrak{D}' . First recall some well-known facts about torsion-free symplectic connections on (M, ω) . Given two such connections ∇ and ∇' , it is obvious that $S^{\nabla-\nabla'}(X, Y) := \nabla_X Y - \nabla'_X Y$, where $X, Y \in \Gamma^\infty(TM)$ defines a symmetric tensor field $S^{\nabla-\nabla'} \in \Gamma^\infty(\bigvee^2 T^*M \otimes TM)$ on M . Defining $\sigma^{\nabla-\nabla'}(X, Y, Z) := \omega(S^{\nabla-\nabla'}(X, Y), Z)$ it is easy to see that $\sigma^{\nabla-\nabla'} \in \Gamma^\infty(\bigvee^3 T^*M)$ is a totally symmetric tensor field. Conversely, given an arbitrary element $\sigma \in \Gamma^\infty(\bigvee^3 T^*M)$ and a symplectic torsion-free connection ∇ and defining $S^\sigma \in \Gamma^\infty(\bigvee^2 T^*M \otimes TM)$ by $\sigma(X, Y, Z) = \omega(S^\sigma(X, Y), Z)$, then ∇^σ defined by $\nabla^\sigma_X Y := \nabla_X Y - S^\sigma(X, Y)$ again is a torsion-free symplectic connection and all such connections can be obtained this way by varying σ . Using these relations, one can compare the corresponding mappings ∇ and ∇' on $\mathcal{W} \otimes \Lambda$. With the notations from above we have

$$\begin{aligned} \nabla - \nabla' &= -(dx^i \otimes dx^j) i_s(S^{\nabla-\nabla'}(\partial_i, \partial_j)) \\ &= \frac{1}{\nu} \text{ad}(T^{\nabla-\nabla'}) \end{aligned} \quad [29]$$

where $T^{\nabla-\nabla'} \in \Gamma^\infty(\bigvee^2 T^*M \otimes T^*M) \subseteq \mathcal{W} \otimes \Lambda^1$ is defined by $T^{\nabla-\nabla'}(Z, Y; X) := \sigma^{\nabla-\nabla'}(X, Y, Z) = \omega(S^{\nabla-\nabla'}(X, Y), Z)$. Moreover, $T^{\nabla-\nabla'}$ satisfies the equations

$$\delta T^{\nabla-\nabla'} = 0 \quad [30a]$$

and

$$\begin{aligned} \nabla T^{\nabla-\nabla'} &= R' - R + \frac{1}{\nu} T^{\nabla-\nabla'} \circ T^{\nabla-\nabla'} \\ \nabla' T^{\nabla-\nabla'} &= R' - R - \frac{1}{\nu} T^{\nabla-\nabla'} \circ T^{\nabla-\nabla'} \end{aligned} \quad [30b]$$

where $R = (1/4)\omega_{it}R^t_{jkl}dx^i \vee dx^j \otimes dx^k \wedge dx^l$ and $R' = (1/4)\omega_{it}R'^t_{jkl}dx^i \vee dx^j \otimes dx^k \wedge dx^l$ denote the corresponding elements of $\mathcal{W} \otimes \Lambda^2$ that are built from the curvature tensors of ∇ and ∇' .

Now we are in the position to compare two Fedosov derivations \mathfrak{D} and \mathfrak{D}' resp. the induced star products $*$ and $*$ ' obtained from (∇, Ω) and (∇', Ω') . The idea for the construction of an equivalence transformation from $*$ to $*$ ' is to look for an automorphism \mathcal{A}_h of $(\mathcal{W} \otimes \Lambda, \circ)$ of the form

$$\mathcal{A}_h = \exp\left(\frac{1}{\nu} \text{ad}(h)\right) \text{ such that } \mathfrak{D}' = \mathcal{A}_h \mathfrak{D} (\mathcal{A}_h)^{-1} \quad [31]$$

where h is an element of \mathcal{W}_3 guaranteeing that \mathcal{A}_h is well defined and without loss of generality is assumed to satisfy $\sigma(h) = 0$. In case one can find such an element h it is clear that \mathcal{A}_h yields a bijection between

$\ker(\mathfrak{D}) \cap \mathcal{W}$ and $\ker(\mathfrak{D}') \cap \mathcal{W}$ and hence one would obtain an equivalence S_h from $*$ to $*$ ' defining

$$\begin{aligned} S_h f &:= \sigma(\mathcal{A}_h \tau(f)) \\ &= \sigma\left(\exp\left(\frac{1}{\nu} \text{ad}(h)\right) \tau(f)\right) \end{aligned} \quad [32a]$$

with inverse

$$\begin{aligned} (S_h)^{-1} f &= \sigma((\mathcal{A}_h)^{-1} \tau'(f)) \\ &= \sigma\left(\exp\left(-\frac{1}{\nu} \text{ad}(h)\right) \tau'(f)\right) \end{aligned} \quad [32b]$$

A direct computation yields

$$\mathcal{A}_h \mathfrak{D} (\mathcal{A}_h)^{-1} = \mathfrak{D} - \frac{1}{\nu} \text{ad}\left(\frac{\exp((1/\nu)\text{ad}(h)) - \text{id}}{(1/\nu)\text{ad}(h)}(\mathfrak{D}h)\right)$$

which is equal to \mathfrak{D}' iff h has been chosen such that

$$T^{\nabla-\nabla'} + r' - r - \frac{\exp((1/\nu)\text{ad}(h)) - \text{id}}{(1/\nu)\text{ad}(h)}(\mathfrak{D}h) \in \mathcal{W} \otimes \Lambda^1 \quad [33]$$

is a central element. Considering the total degree of the terms in this expression, this is the case iff there is a formal series of 1-forms $C \in \nu\Gamma^\infty(T^*M)[[\nu]]$ such that the expression in eqn [33] equals $1 \otimes C$. Applying \mathfrak{D} to this equation and using the equations that r and r' satisfy together with the relations [30] it is cumbersome but not difficult to show that necessarily Ω and Ω' have to be cohomologous:

$$\Omega - \Omega' = dC \quad [34]$$

with C as above. Now, using [6] one can show that this condition is in fact sufficient and moreover one can even determine the element h in question recursively:

Theorem 5 (Fedosov 1994, theorem 4.3). *Two Fedosov star products $*$ and $*$ ' obtained from (∇, Ω) and (∇', Ω') are equivalent iff Ω and Ω' are cohomologous. In case $C \in \nu\Gamma^\infty(T^*M)[[\nu]]$ satisfies $\Omega - \Omega' = dC$ there is a uniquely determined element $h_C \in \mathcal{W}_3$ with $\sigma(h_C) = 0$ such that*

$$T^{\nabla-\nabla'} + r' - r - \frac{\exp((1/\nu)\text{ad}(h_C)) - \text{id}}{(1/\nu)\text{ad}(h_C)}(\mathfrak{D}h_C) = 1 \otimes C$$

Moreover, h_C can be determined recursively from

$$\begin{aligned} h_C &= C \otimes 1 + \delta^{-1}\left(\nabla h_C - \frac{1}{\nu} \text{ad}(r)h_C \right. \\ &\quad \left. - \frac{(1/\nu)\text{ad}(h_C)}{\exp((1/\nu)\text{ad}(h_C)) - \text{id}}(r' - r + T^{\nabla-\nabla'})\right) \end{aligned} \quad [35]$$

and with the so-constructed h_C one has $\mathcal{D}' = A_{h_C} \mathcal{D} (A_{h_C})^{-1}$ and thus S_{h_C} according to eqn [32] defines an equivalence transformation from $*$ to $*'$.

Evidently, in the above construction of the equivalence transformation S_{h_C} there is some choice of the formal series of 1-forms C . Different possible choices C and \tilde{C} differ by a formal series of closed 1-forms but choosing \tilde{C} instead of C amounts to another equivalence transformation $S_{h_{\tilde{C}}} = A' S_{h_C} A$ from $*$ to $*'$, where A and A' are certain self-equivalences of $*$ and $*'$, respectively. In case Ω and Ω' are real, we have seen that $*$ as well as $*'$ are Hermitian star products and it is easy to verify that choosing a formal series C of 1-forms as above that is moreover real yields an element h_C satisfying $\overline{h_C} = h_C$. But then it is evident that the resulting equivalence transformation is also compatible with complex conjugation, that is, $\overline{S_{h_C} f} = S_{h_C} \bar{f}$ for all $f \in \mathcal{C}^\infty(M)[[\nu]]$.

Now we are prepared to give a construction of all $\mathbb{C}[[\nu]]$ -linear automorphisms of a Fedosov star product $*$. It is easy to show that any $\mathbb{C}[[\nu]]$ -linear automorphism of a star product $*$ on a symplectic manifold is the combination of the action of a symplectomorphism $\psi: M \rightarrow M$ and an equivalence between $*$ and the pullback $*'$ via ψ^{-1} of $*$, which is defined by $f \star' g = (\psi^{-1})^*((\psi^* f) \star (\psi^* g))$ (cf. Gutt and Rawnsley (1999 Proposition 9.4)). Since the characteristic class of $*'$ is given by $c(*') = (\psi^{-1})^* c(*)$, the necessary and sufficient condition for a symplectomorphism ψ to define a possible zeroth-order term of an automorphism is that $(\psi^{-1})^* c(*) = c(*)$ since $*'$ and $*$ have to be equivalent.

Within Fedosov's framework, it can be shown that the pullback $*'$ via a symplectomorphism ψ^{-1} of $*$ is identical to the Fedosov star product obtained from $(\nabla' = (\psi^{-1})^* \nabla \psi^*, \Omega' = (\psi^{-1})^* \Omega)$, which just expresses the functoriality of Fedosov's construction. Together with Theorem 4 this particularly shows that $c(*') = (\psi^{-1})^* c(*)$, and therefore $*'$ is equivalent to $*$ iff Ω and Ω' differ by a formal series dC_ψ of exact 2-forms, where $C_\psi \in \nu \Gamma^\infty(T^*M)[[\nu]]$ clearly depends on ψ . But in this situation one can apply the construction of equivalence transformations between Fedosov star products given in Theorem 5 with C replaced by C_ψ and ∇', Ω' as above yielding an equivalence $S_{h_\psi} := S_{h_{C_\psi}}$ from $*$ to $*'$. Finally, we therefore get that the combination

$$A_\psi := \psi^* S_{h_\psi} \quad [36]$$

is a $\mathbb{C}[[\nu]]$ -linear automorphism of $*$ and it is obvious from the above that every such automorphism can be obtained by considering all symplectomorphisms ψ of (M, ω) satisfying $[(\psi^{-1})^* \Omega] = [\Omega]$ and

composing the resulting A_ψ according to [36] with all self-equivalences A of $*$ according to [28].

Adaptions, Modifications, and Generalizations

The geometrical construction of Fedosov has gone through many adaptions and modifications that are well suited to the particular geometry of the underlying symplectic manifold. Moreover, there are generalizations that go beyond the case of symplectic manifolds and others that yield more general deformations than star products. We just give a few important examples that stress the power and beauty of Fedosov's construction.

On a Kähler manifold, one can define the notion of star products with separation of variables (cf. Karabegov (1996) that are also called star products of Wick type (cf. Bordemann and Waldmann (1997) and Neumaier (2003)). These are star products such that in local holomorphic coordinates the bidifferential operators C_r are of the form

$$C_r(f, g) = \sum_{K, \bar{L}} C_r^{K, \bar{L}} \frac{\partial^{|K|} f}{\partial z^K} \frac{\partial^{\bar{L}} g}{\partial \bar{z}^{\bar{L}}} \quad [37]$$

with certain coefficient functions $C_r^{K, \bar{L}}$. These star products can be obtained by a modified Fedosov construction starting from the product \circ_{Wick} on $\mathcal{W} \otimes \Lambda$ given by

$$a \circ_{\text{Wick}} b = \mu \left(\exp \left(\frac{2\nu}{i} g^{k\bar{l}} i_s(\partial_{z_k}) \otimes i_{\bar{s}}(\partial_{\bar{z}_l}) \right) (a \otimes b) \right) \quad [38]$$

where $g^{k\bar{l}}$ denotes the components of the inverse of the Kähler metric in local holomorphic coordinates. In the case of a Kähler manifold, there is a distinguished torsion-free symplectic connection namely the Kähler connection ∇ that induces a superderivation of \circ_{Wick} in a way completely analogous to [8]. With these structures the Fedosov construction works for an arbitrary formal series Ω of closed 2-forms as before, but one can show that the resulting star product is of Wick type iff Ω is of type (1, 1) and one can even show that one obtains all star products of Wick type by varying Ω (cf. Neumaier (2003)).

In the case of an almost-Kähler manifold, one can consider a product \circ' on $\mathcal{W} \otimes \Lambda$ similar to \circ_{Wick} which is adapted to the almost-complex structure (cf. Karabegov and Schlichenmaier (2001)). However, in this situation there is no torsion-free connection that yields a superderivation of this product but only a connection ∇' with torsion that defines such a superderivation. Nevertheless, one

can consider a generalized Fedosov construction. To this end, one shows that $[\delta, \nabla'] = (1/\nu)\text{ad}'(T')$ with some $T' \in \mathcal{W} \otimes \Lambda^2$ that satisfies $\delta T' = 0$ and encodes the torsion of ∇' and $\delta R' = \nabla' T'$, where again $\nabla'^2 = -(1/\nu)\text{ad}'(R')$ and R' , which depends on the curvature of ∇' , satisfies $\nabla' R' = 0$. But then it is easy to show that there is a unique element $r' \in \mathcal{W}_2 \otimes \Lambda^1$ such that

$$\delta r' = \nabla' r' - \frac{1}{\nu} r' \circ' r' + T' + R' + 1 \otimes \Omega$$

and

$$\delta^{-1} r' = 0 \quad [39]$$

with Ω as above, which can also be computed recursively. Clearly, $\mathfrak{D}' = -\delta + \nabla' - (1/\nu)\text{ad}'(r')$ then is a suitable Fedosov derivation with square zero for \circ' and one can proceed as described earlier to obtain a star product \ast' adapted to the almost-complex structure.

On a cotangent bundle $\pi: T^*Q \rightarrow Q$, where T^*Q is equipped with the canonical symplectic form $\omega_0 = -d\theta_0$, one can consider (cf. Bordemann *et al.* (1998)) the following so-called standard ordered product \circ_{std} on $\mathcal{W} \otimes \Lambda$ given by

$$a \circ_{\text{std}} b = \mu \left(\exp \left(-\nu i_s(\partial_{p_i}) \otimes i_s(\partial_{q^i} + p_l \pi^* \Gamma_{ik}^l \partial_{p_k}) \right) \times (a \otimes b) \right) \quad [40]$$

in local Darboux coordinates. Here Γ_{ik}^l denotes the Christoffel symbols of a torsion-free connection ∇^Q on Q in the chart of Q corresponding to the bundle chart (q, p) and it is straightforward to see that \circ_{std} does not depend on the chosen local coordinates and is associative. In the present situation, one can define a torsion-free symplectic connection ∇^{T^*Q} on T^*Q solely in terms of ∇^Q but then the corresponding mapping ∇^{T^*Q} on $\mathcal{W} \otimes \Lambda$ again fails to be a superderivation of \circ_{std} , whereas the combination $\nabla^{T^*Q} + \mathcal{B}$ with $\mathcal{B} = (\nu/3) p_l \pi^* R_{jik}^l (1 \otimes dq^i) i_s(\partial_{p_j}) i_s(\partial_{p_k})$, where R_{jik}^l denotes the components of the curvature tensor of ∇^Q , turns out to be a suitable superderivation to start the Fedosov construction with \circ_{std} . In fact, the square of $\nabla^{T^*Q} + \mathcal{B}$ turns out to equal the square of ∇^{T^*Q} and all the other preconditions of Fedosov's construction are easily verified just replacing ∇ by $\nabla^{T^*Q} + \mathcal{B}$. The particular property of the resulting star product \ast_{std} for $\Omega = 0$ on T^*Q is that it is a standard ordered star product, that is, for all $f \in C^\infty(T^*Q)[[\nu]]$ and all $\chi \in C^\infty(Q)[[\nu]]$ one has

$$\pi^* \chi \ast_{\text{std}} f = \pi^* \chi f \quad [41]$$

and hence \ast_{std} in a certain sense is adapted to the vertical polarization.

The methods mentioned so far can even be melted into a more general situation, where one considers a (complex) polarization on (M, ω) and looks for star products that are adapted to this polarization which are then called polarized deformation quantizations (cf. Donin (2003)). Here again a generalization of Fedosov's construction yields the existence and the classification of such particular star products.

Another recent generalization of Fedosov's construction that goes beyond the framework of smooth symplectic manifolds is that of the construction of star products on symplectic orbispaces (cf. Pflaum (2003)), which are stratified symplectic spaces. The main idea there is to consider Fedosov's construction in local orbicharts and to show that the changes of orbicharts induce isomorphisms between the locally defined deformation quantizations, implying that the locally defined products match together to define a global deformation quantization on the symplectic orbispace. To achieve this property, one has to adjust the local Fedosov constructions appropriately, that is, one has to use locally defined torsion-free symplectic connections and formal series of closed 2-forms that are related by the changes of the orbicharts.

Considering a vector bundle $E \rightarrow M$, the sections $\Gamma^\infty(E)$ are naturally a $C^\infty(M)$ -right module and a $\Gamma^\infty(\text{End}(E))$ -left module, and it is a natural question whether this bimodule structure can be deformed such that $\Gamma^\infty(E)[[\nu]]$ becomes a $(C^\infty(M)[[\nu]], \star)$ -right module and a $(\Gamma^\infty(\text{End}(E)[[\nu]], \star)$ -left module, where \star is a deformation of the usual composition of elements of $\Gamma^\infty(\text{End}(E))$. In order to construct such deformations, one can also adapt Fedosov's construction (cf. Waldmann (2002)) considering $\mathcal{W} \otimes \Lambda \otimes \mathcal{E} = (\mathbf{X}_{s=0}^\infty \Gamma^\infty(\bigvee^s T^*M \otimes \bigwedge T^*M \otimes E))[[\nu]]$ and $\mathcal{W} \otimes \Lambda \otimes \text{End}(\mathcal{E}) = (\mathbf{X}_{s=0}^\infty \Gamma^\infty(\bigvee^s T^*M \otimes \bigwedge T^*M \otimes \text{End}(E)))[[\nu]]$ and extending the product \circ to these spaces in a natural way making $\mathcal{W} \otimes \Lambda \otimes \mathcal{E}$ a $(\mathcal{W} \otimes \Lambda \otimes \text{End}(\mathcal{E}), \circ) - (\mathcal{W} \otimes \Lambda, \circ)$ -bimodule. Furthermore, one has to consider a connection ∇^E that naturally induces a connection on $\text{End}(E)$, and both have to be added to ∇ to define the corresponding substitute of ∇ on the respective space. Then the Fedosov construction with $\mathcal{W} \otimes \Lambda \otimes \text{End}(\mathcal{E})$ can be considered yielding a Fedosov derivation $\mathfrak{D}^{\text{End}(E)}$ with square zero, hence a Fedosov–Taylor series $\tau^{\text{End}(E)}$ and an associative deformation $F \# G = \sigma(\tau^{\text{End}(E)}(F) \circ \tau^{\text{End}(E)}(G))$ of the usual composition of sections in the endomorphism bundle. Moreover, there is a map \mathfrak{D}^E on $\mathcal{W} \otimes \Lambda \otimes \mathcal{E}$ that is a superderivation with respect to the bimodule multiplication \circ along $\mathfrak{D}^{\text{End}(E)}$ and \mathfrak{D} , respectively. This map also has square zero and the intersection of its kernel with the elements of antisymmetric degree is in bijection to $\Gamma^\infty(E)[[\nu]]$ via a natural generalization τ^E of the Fedosov–Taylor

series. Defining $F \odot s := \sigma(\tau^{\text{End}(E)}(F) \circ \tau^E(s))$ and $s \cdot f := \sigma(\tau^E(s) \circ \tau(f))$, $\Gamma^\infty(E)[[\nu]]$ can be given the structure of a $(\Gamma^\infty(\text{End}(E))[[\nu]], \#) - (C^\infty(M)[[\nu]], *)$ -bimodule which is indeed a deformation of the classical bimodule structure of $\Gamma^\infty(E)$. It is rather evident that the same procedure also works for other products on $\mathcal{W} \otimes \Lambda$ and the above generalizations, in particular for the product \circ_{Wick} on a Kähler manifold, where one can obtain $(\Gamma^\infty(\text{End}(E))[[\nu]], \#_{\text{Wick}}) - (C^\infty(M)[[\nu]], *_\text{Wick})$ -bimodules that are adapted to the complex structure in case the curvature endomorphism of the connection ∇^E is of type $(1, 1)$. For example, this holds true for (anti-) holomorphic vector bundles endowed with a Hermitian fiber metric h and the corresponding connection that is compatible with h and the (anti-) holomorphic structure.

Finally, the proof of existence of deformation quantizations on arbitrary Poisson manifolds (M, Π) , that includes a concrete construction starting from Kontsevich's star product on the flat space \mathbb{R}^n equipped with a Poisson tensor, given by Cattaneo *et al.* (2002) is similar in spirit to Fedosov's construction. There one constructs two bundles J^∞ and \mathcal{J}^∞ of associative algebras, where $-$ as a bundle $-\mathcal{J}^\infty$ is isomorphic to $J^\infty[[\nu]]$ and J^∞ is the bundle of infinite jets of smooth functions on M which is equipped with the canonical flat connection D_0 . The Poisson tensor gives rise to the structure of a Poisson algebra on each fiber of J^∞ and the canonical map $C^\infty(M) \rightarrow J^\infty$ yields a Poisson algebra isomorphism between $C^\infty(M)$ and the Poisson algebra of D_0 -flat sections in J^∞ . The second step in the construction consists in a deformation of this correspondence. Using the Kontsevich formula for \mathbb{R}^n , each fiber of \mathcal{J}^∞ can be equipped with an associative product which is a deformation of the above product on the fibers of J^∞ in the direction of the Poisson bracket induced by Π . Then analogously to Fedosov's construction, one constructs a compatible connection $D = D_0 + \nu D_1 + \nu^2 D_2 + \dots$ which is a deformation of D_0 . Here compatibility just means that D is a derivation with respect to the above product on sections in \mathcal{J}^∞ implying that the D -flat sections form a subalgebra. Moreover, one can achieve that this connection is flat and in this case $C^\infty(M)[[\nu]]$ turns out to be in bijection to the D -flat sections in \mathcal{J}^∞ . For the proof of existence of D and for its recursive determination using an adaption of Fedosov's method, again special cases of Kontsevich's formality theorem prove to be the crucial tools. Pulling back the above fiberwise product to $C^\infty(M)[[\nu]]$ via this isomorphism, one then obtains a star product on (M, Π) . Since this isomorphism can be determined recursively, the star product can in principle be computed explicitly.

See also: Deformation Quantization; Deformation Quantization and Representation Theory; Deformation Theory; Deformations of the Poisson Bracket on a Symplectic Manifold; String Field Theory.

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Feigenbaum Phenomenon see Universality and Renormalization

Fermionic Systems

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Quantum Statistics

Quantum particles are described by a complex, square-integrable wave function $\Psi(x_1, \dots, x_N)$ with $|\Psi|^2$ representing the probability density of finding N particles at positions x_1, x_2, \dots, x_N , which will be assumed to be in a d -dimensional square box V with side L and periodic boundary conditions. If the N particles are identical, $|\Psi|^2$ must be totally symmetric in the exchange of any pair of coordinates. Regarding the symmetry properties of Ψ itself, it is an experimental fact (which finds its theoretical explanation in the context of relativistic quantum field theory) that only two possibilities can arise: either Ψ is symmetric or it is antisymmetric, which means that $\Psi(x_1, \dots, x_N) = (-1)^P \Psi(x_{P_1}, \dots, x_{P_N})$, where P_1, \dots, P_N is a permutation of $1, \dots, N$, and $(-1)^P$ is the parity of the permutation. Particles described by a symmetric wave function are called bosons, while particles with an antisymmetric wave function are called fermions, after Bose and Fermi, who introduced these concepts. The fermionic wave function therefore vanishes if two coordinates are equal, a property called Pauli exclusion principle. Particles have an intrinsic quantized angular momentum called spin and particles with semi-integer spin are fermions, while particles with integer spin are bosons. Examples of fermions are electrons, protons, or neutrons, with spin $\sigma = \pm \hbar/2$, where \hbar is the Planck constant; examples of bosons are phonons or mesons with integer spin.

The time evolution of a wave function is driven (through the Schrödinger equation) by the Hamiltonian operator, and the choice of such an operator is determined by the physical system we want to

describe. One of the most important physical realizations of a fermionic system is given by the conduction electrons in solids with a crystalline structure (like metals). According to the classical theory of Drude, a crystal can be described as a lattice of atoms in which the valence electrons are lost by the atoms (which become ions) and move freely in the metal; they are responsible for the conduction properties of the crystal. However, if one assumes that the electrons are classical particles (in the sense that they obey the Newtonian mechanics), one obtains wrong predictions about the properties of crystals. One has to take into account that the conduction electrons are quantum particles and this provides us with a natural example of a fermionic system; the Hamiltonian can be taken as

$$H_N = \sum_{i=1}^N \left[-\frac{\hbar^2 \partial_{x_i}^2}{2m} + uc(x_i) \right] + \sum_{i < j} \lambda v(x_i - x_j) \quad [1]$$

The first term represents the nonrelativistic kinetic energy of the electrons (m is the mass), $uc(x)$ is a periodic potential due to the ions in the lattice ($c(x) = c(x + R)$ with $R = (n_1 a_1, \dots, n_d a_d)$, $n_i \in \mathbb{Z}$) and $\lambda v(x - y)$ is a two-body interaction potential, which is modeled by a short-range potential to take into account, phenomenologically, the electrostatic screening. Finally, λ and u are couplings which measure the "strength" of the corresponding interaction. Much more complicated and "realistic" Hamiltonians could be considered; for instance, one can add an interaction with a stochastic field to take into account impurities in the lattice, or with a boson field to take into account the dynamics of the ions, and so on. Note also that one can study not only three-dimensional Fermi systems ($d=3$), but also $d=2$ or $d=1$ systems; they can describe the conduction electrons of crystals that are anisotropic and should be considered as bidimensional or one-dimensional systems. We focus on the nonrelativistic

fermionic systems with Hamiltonian [1], which is a problem of great importance from both the conceptual and the applications point of view.

Second-Quantization Formalism

The Hilbert space of states of a system of $N > 1$ fermions is the space \mathcal{H}_N of all the complex square-integrable antisymmetric functions $\Psi(\mathbf{x}_1, \dots, \mathbf{x}_N)$. Let $\{\phi_k(\mathbf{x})\}_{k \in \mathbb{R}^d}$ be a basis for \mathcal{H}_1 (the one-particle Hilbert space of all the complex square-integrable functions $\Psi(\mathbf{x}_1)$), where k is an index called quantum number. Usually, the set of $\phi_k(\mathbf{x})$ is chosen as the eigenfunctions of the single-particle Hamiltonian

$$-\frac{\hbar^2 \partial_x^2}{2m} + u c(\mathbf{x})$$

for instance, if $u = 0$ then

$$\phi_k(\mathbf{x}) = \frac{1}{L^{d/2}} e^{i\mathbf{k}\mathbf{x}}$$

with $\hbar k$ representing the momentum; due to periodic boundary conditions, k has the form $k = (2\pi/L)\mathbf{n}$, $\mathbf{n} = n_1, \dots, n_d$ with n_i integer and $-[L/2] \leq n_i \leq [L/2]$. If we call $|k_1, \dots, k_N\rangle$ the normalized antisymmetrization of $\phi_{k_1}(\mathbf{x}_1)\phi_{k_2}(\mathbf{x}_2)\dots\phi_{k_N}(\mathbf{x}_N)$ (Slater determinant), then the set of all possible $|k_1, \dots, k_N\rangle$ is a basis for \mathcal{H}_N ; $|k_1, \dots, k_N\rangle$ describes a state in which the N fermions have quantum numbers k_1, \dots, k_N . One can introduce (Negele and Orland 1988, Berezin 1966) the creation or annihilation operators a_k^+, a_k^- : they are anticommuting operators,

$$\begin{aligned} \{a_k^+, a_{k'}^-\} &\equiv a_k^+ a_{k'}^- + a_{k'}^- a_k^+ = \delta_{k,k'} \\ \{a_k^+, a_{k'}^+\} &= \{a_k^-, a_{k'}^-\} = 0 \end{aligned} \quad [2]$$

such that $a_k^+ |k_1, \dots, k_N\rangle = |k, k_1, \dots, k_N\rangle$ if $k \neq k_i$, $i = 1, \dots, N$ and 0 otherwise; a_k^- is the adjoint of a_k^+ . The action of a_k^+ is to create a particle with quantum number k if it is not present in the state, and to yield zero otherwise (according to the Pauli principle). The state $|0\rangle$ such that $a_k^- |0\rangle = 0$ for all k is called the vacuum state and it represents a state with no particles. The Fock space is defined as the direct sum of the Hilbert spaces with any number of particles, and all the elements of the Fock space can be generated by linearly superposing products of creation operators acting over the vacuum state. We can extend such definitions by adding a label to such operators to take into account the spin of the particle; for example, $a_{k,\sigma}^\pm$ are creation or annihilation operators of a particle with spin σ and position k . In terms of $a_{x,\sigma}^\pm = L^{-d/2} \sum_k \phi_k(\mathbf{x}) a_{k,\sigma}^\pm$ and of its adjoint $a_{x,\sigma}^-$, the Hamiltonian can be written as

$$\begin{aligned} H = & \sum_\sigma \left[\int_V d\mathbf{x} a_{x,\sigma}^+ \frac{-\hbar^2 \partial_x^2}{2m} a_{x,\sigma}^- \right. \\ & \left. + u \int_V d\mathbf{x} c(\mathbf{x}) a_{x,\sigma}^+ a_{x,\sigma}^- \right] \\ & + \sum_{\sigma,\sigma'} \lambda \int_V d\mathbf{x} \int_V d\mathbf{y} v(\mathbf{x} - \mathbf{y}) a_{x,\sigma}^+ a_{x,\sigma}^- a_{y,\sigma'}^+ a_{y,\sigma'}^- \quad [3] \end{aligned}$$

According to the postulates of quantum statistical mechanics, the grand canonical partition function is given by $Z = \text{tr} e^{-\beta(H - \mu N)}$, where $\beta = (\kappa T)^{-1}$, κ is the Boltzmann constant, T is the temperature, μ is the chemical potential, $N = \sum_\sigma \int d\mathbf{x} a_{x,\sigma}^+ a_{x,\sigma}^-$, and tr is the trace operation over the Fock space. The thermodynamical average of an observable O is given by $\langle O \rangle = Z^{-1} \text{tr}[e^{-\beta(H - \mu N)} O]$. Given a fermionic system, one is often interested in its Schwinger functions defined as follows: if $\mathbf{x} = (\mathbf{x}, t)$ and $t_1 \geq t_2 \geq \dots \geq t_s$, s even, then

$$\begin{aligned} S(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_s) &= \frac{\text{tr} e^{-(\beta - t_1)(H - \mu N)} \psi_{x_1}^{\varepsilon_1} e^{-(t_1 - t_2)(H - \mu N)} \psi_{x_2}^{\varepsilon_2} \dots e^{-t_s(H - \mu N)}}{\text{tr} e^{-\beta(H - \mu N)}} \quad [4] \end{aligned}$$

with $\varepsilon_i = \pm$, $-\beta/2 \leq t_i \leq \beta/2$; periodic and anti-periodic boundary conditions are, respectively, imposed over x_i and t_i . From the knowledge of the Schwinger functions, one can compute all the thermodynamical properties of a system at equilibrium or close to equilibrium.

The Free Fermi Gas

Computation of the physical observables corresponding to the complete Hamiltonian [3] is a very difficult task. The natural starting point consists in taking into account only the kinetic term by putting $\lambda = u = 0$ in [3], obtaining the free Fermi gas model. The resulting model is not trivial at all; its properties are radically different with respect to the ones of a gas of classical particles, and it is sufficient to understand many properties of matter (see, e.g., Mahan (1990)). If

$$\phi_k(\mathbf{x}) = \frac{1}{L^{d/2}} e^{i\mathbf{k}\mathbf{x}}$$

then $|k_1, \sigma_1, \dots, k_N, \sigma_N\rangle$ are eigenfunctions of H with eigenvalue $\sum_{k,\sigma} \varepsilon(k) n_{k,\sigma}$, where $\varepsilon(k) = \hbar^2 |k|^2 / 2m$ and $n_{k,\sigma} = 0, 1$, the occupation number, is the eigenvalue $a_{k,\sigma}^+ a_{k,\sigma}^-$; $n_{k,\sigma} = 1$ if in the state there is a fermion with momentum k and spin σ , and it is zero otherwise. The eigenfunction $|\Omega\rangle$ of H with lowest energy is called the ground state, and it determines the low-temperature properties of the system. In order to find the ground state $|\Omega\rangle$, one has

to minimize $\sum_{k,\sigma} \varepsilon(k) n_{k,\sigma}$ with the constraint that $n_{k,\sigma}$ can take only the values 0 or 1 and $\sum_{k,\sigma} n_{k,\sigma} = N$; if there are many solutions to this problem, one says that the ground state is degenerate. An approximate solution is the following: if $d=3$, one can consider a state such that $n_{k,\sigma} = 1$ if \mathbf{k} is in a sphere of radius k_F and zero otherwise; since the number of momenta $\mathbf{k} = (2\pi/L)\mathbf{n}$ in the sphere is approximately given by

$$2 \frac{4\pi k_F^3}{3} \frac{L^3}{8\pi^2}$$

we can choose $k_F = (3\pi^2 \rho)^{1/3}$, with $\rho = NL^{-3}$. The state $\prod_{|\mathbf{k}| \leq k_F} a_{1/2, \mathbf{k}}^+ a_{-1/2, \mathbf{k}}^+ |0\rangle$ is not the true ground state when N, L are finite, but it is a very good approximation of it and converges to it (in a suitable sense) in the limit $N, L \rightarrow \infty$, ρ fixed. The boundary of the sphere with radius k_F in the space of momenta is called the Fermi surface, and it is a key notion in the theory of Fermi systems; if $d=2$, it is replaced by a circle and in $d=1$ by two points.

Coming to the thermodynamical properties, the partition function is given by

$$Z = \prod_k \sum_{n_k=0,1} e^{-\beta(\varepsilon(k)-\mu)n_k} = \prod_k (1 + e^{-\beta(\varepsilon_k - \mu)})$$

and the specific heat by

$$C_v = -\frac{\partial}{\partial T} \frac{\partial}{\partial \beta} \log Z$$

One finds, by expressing μ in terms of β through the relation $N = -\partial f / \partial \mu$, that if $d=3$, in the $L \rightarrow \infty$ limit

$$C_v = \frac{\pi^2}{2} \rho \kappa \left(\frac{\kappa T}{\varepsilon_F} \right) + O\left(\frac{\kappa T}{\varepsilon_F} \right)^2$$

where $\varepsilon_F = \hbar^2 k_F^2 / 2m$. Early models for metals described the electrons as classical particles; however in such a case, a well-known result of classical statistical mechanics states that they should contribute to the specific heat by $\frac{3}{2} \rho \kappa$, while experimentally their contribution is much smaller. The solution of this puzzle was provided by the above formula for C_v ; the classical value is in fact depressed by a factor

$$\frac{\pi^2}{3} \frac{\kappa T}{\varepsilon_F}$$

which at room temperatures is $O(10^{-2})$, in agreement with experimental data. The average number of electrons with momentum $\hbar \mathbf{k}$ is given, in the infinite-volume limit, by

$$\langle a_{k,\sigma}^+ a_{k,\sigma}^- \rangle = (1 + e^{\beta(\varepsilon(k)-\mu)})^{-1}$$

At zero temperature, it reduces to $\theta(|\mathbf{k}| \leq k_F)$, that is, it has a discontinuity at the Fermi surface, while

at high temperatures it is very close to the Maxwell distribution $\simeq e^{-\beta(\varepsilon(k)-\mu)}$.

Finally, in the free Fermi gas model, all Schwinger functions can be computed. One finds that, if, for instance, $\varepsilon_i = +$ for $i=1, 2, \dots, s/2$ and $\varepsilon_i = -$ otherwise, that the Schwinger function with $s \geq 4$ can be expressed as sum of products of the $s=2$ Schwinger function (also called the propagator)

$$S(x_1, \dots, x_s) = \sum_{\pi} (-1)^{\pi} \prod_{i,j} S_0(x_i - x_{\pi(j)}) \quad [5]$$

where $i=1, \dots, s/2$, $j=s/2+1, \dots, s$, π_j is a permutation of $j=s/2+1, \dots, s$, $(-1)^{\pi}$ is the parity of this permutation, \sum_{π} is the sum over all the possible permutations; such a formula is called the Wick rule. By an explicit computation, $S_0(x-y)$ is given by

$$\begin{aligned} & \frac{2\pi}{\beta} \sum_{k_0=2\pi(n_0+1/2)\beta^{-1}} \left(\frac{2\pi}{L} \right)^d \sum_{\mathbf{k}=(2\pi/L)\mathbf{n}} \frac{e^{ik(x-y)}}{-ik_0 + |\mathbf{k}|^2/2m - \mu} \\ & \equiv \frac{2\pi}{\beta} \sum_{k_0=2\pi(n_0+1/2)\beta^{-1}} \left(\frac{2\pi}{L} \right)^d \sum_{\mathbf{k}=(2\pi/L)\mathbf{n}} e^{ik(x-y)} \hat{S}_0(\mathbf{k}) \end{aligned} \quad [6]$$

where $\mathbf{k} = (k_0, \mathbf{k})$. In the limit $L, \beta \rightarrow \infty$, for large distances $S(x, y)$ decays as a power law, $O(|x-y|^{-1})$ times an oscillating function of period k_F^{-1} . Note that $S_0(\mathbf{k})$ in the limit $\beta, L \rightarrow \infty$ diverges for $k_0=0$ and $\varepsilon(\mathbf{k})=\mu$, that is, at the Fermi surface ($\mu=\varepsilon_F$ in the limit $\beta \rightarrow \infty$); when β is finite, $S_0(\mathbf{k})$ is finite even for $L \rightarrow \infty$, that is, the finite temperature acts as an infrared cutoff.

Fermions in an External Potential

The next step consists in adding an external periodic potential to the free Fermi gas model, taking into account the field generated by the ions of the lattice. We consider then [3] with $\lambda=0$ and $u \neq 0$. As in the previous case, the eigenfunctions of the N -particle Hamiltonian can be computed and are expressed in terms of the single-particle eigenfunctions of $-\hbar^2 \partial_x^2 / 2m + uc(x)$; they are called Bloch waves and have the form

$$\phi_{\mathbf{k}}(\mathbf{x}) = \frac{1}{\sqrt{L^{d/2}}} e^{ikx} u_{\mathbf{k}}(\mathbf{x}), \quad u_{\mathbf{k}}(\mathbf{x}) = u_{\mathbf{k}}(\mathbf{x} + \mathbf{R})$$

\mathbf{k} , called the crystalline momentum, is conserved modulo \mathbf{G} , the vectors of the reciprocal lattice, defined as

$$\mathbf{G} = 2\pi \left(\frac{n_1}{a_1}, \dots, \frac{n_d}{a_d} \right)$$

The eigenvalue $\varepsilon(\mathbf{k})$ of $-\hbar^2 \partial_x^2 / 2m + u c(\mathbf{x})$ associated with a Bloch wave $\phi_{\mathbf{k}}(\mathbf{x})$ has some peculiar properties; in the $L \rightarrow \infty$ limit, one finds that $\varepsilon(\mathbf{k})$ is not a continuous function (unlike the $u=0$ case) but it has gaps, that is, first-order discontinuities. For $d=1$, by a convergent power-series expansion in u , one finds that $\varepsilon(\mathbf{k})$ is a continuous monotonically increasing function except at the points $\pm \pi n/a$, n an integer; at these points $\varepsilon(\mathbf{R})$ is discontinuous and $\varepsilon((n\pi/a)^+) - \varepsilon((n\pi/a)^-) \equiv \Delta_n = u \hat{c}_n + O(u^2)$; the gaps divide $\varepsilon(\mathbf{k})$ into disconnected pieces called energy bands. Something similar happens in $d=2, 3$, in which gaps open for \mathbf{R} such that $G^2 + 2\mathbf{k}G = 0$.

Again, the eigenfunctions of H are given by $|k_1, \sigma_1, \dots, k_N, \sigma_N\rangle$ with eigenvalue $\sum_{k, \sigma} \varepsilon(\mathbf{k}) n_{k, \sigma}$, and the Fermi surface is still defined by the set \mathbf{k} such that $\varepsilon(\mathbf{k}) = \varepsilon_F$ with ε_F determined by the condition $\sum_{\mathbf{k}: \varepsilon(\mathbf{k}) \leq \varepsilon_F} 1 = N$. However, in this case the Fermi surface is not anymore a sphere in $d=3$, but it is in general a polyhedron of a very complex shape. The Schwinger functions are expressed by the Wick rule [5] in terms of the two-point Schwinger functions; they are given by [6] with $e^{ik(x-y)}$ replaced by $\phi_{\mathbf{k}}(\mathbf{x}) \phi_{\mathbf{k}}^*(\mathbf{y})$ and $|\mathbf{k}|^2 / 2m$ replaced by $\varepsilon(\mathbf{k})$. The asymptotic properties of the two-point Schwinger function are quite different with respect to the $u=0$ case. This is easy to see if $d=1$; in the limit $L, \beta \rightarrow \infty$, $S(\mathbf{k})$ is singular if μ does not belong to the interval $[\varepsilon((n\pi/a)^+), \varepsilon((n\pi/a)^-)]$, whereas it is finite if μ belongs to such an interval; in the first case, $S(\mathbf{x}, \mathbf{y})$ decays for large distances as $O(|\mathbf{x} - \mathbf{y}|^{-1})$, whereas in the second case it is $O(e^{-|\Delta_n||\mathbf{x} - \mathbf{y}|})$. This means that, depending on the number of particles (which essentially fixes μ), the Schwinger function has a totally different asymptotic behavior. This fact has important consequences in many physical properties; for instance, the conductivity (which can be computed from the $s=4$ Schwinger function) vanishes if μ belongs to the interval $[\varepsilon((n\pi/a)^+), \varepsilon((n\pi/a)^-)]$. Similar properties hold for $d=2, 3$; hence, from the knowledge of the number of particles and the periodic potential generated by the ions, one can predict if the system is an insulator or a metal.

Note also that the conductivity is infinite in the infinite-volume and zero-temperature limit, when μ does not correspond to a gap; in other words, the electric current in a perfect crystal lattice is not subjected to any dissipation of energy. A finite resistivity is found only if one takes into account deviations from perfect periodicity. To simulate impurities in the lattice, one can add, according to Anderson, to the Hamiltonian an interaction term of the form $\alpha \phi_{\mathbf{x}} \psi_{\mathbf{x}}^+ \psi_{\mathbf{x}}^-$, where $\phi_{\mathbf{x}}$ is a Gaussian stochastic field. A detailed mathematical investigation has been devoted to the properties of

eigenfunctions of $-\hbar^2 \partial_x^2 / 2m + \alpha \phi_{\mathbf{x}}$, where $\phi_{\mathbf{x}}$ is a Gaussian field (see, e.g., Pastur and Figotin (1991)); it is found that if α is large enough in $d=2, 3$ and for any α in $d=1$, the single-particle eigenfunctions are exponentially localized, that is, they decay exponentially at large distances; this implies a finite conductivity. One can also add to the Hamiltonian a term $\beta \phi_{\mathbf{x}}' \psi_{\mathbf{x}}^+ \psi_{\mathbf{x}}^-$, with $\phi_{\mathbf{x}}'$ a quasiperiodic function, in order to describe crystals in which the lattice develops a periodic distortion, with incommensurate period with respect to the lattice periodicity. For $d=1$ and β large, one again finds localized eigenfunctions, whereas for small β there are extended states (see, e.g., Pastur and Figotin (1991)); such results are obtained with the Kolgomorov-Arnol'd-Moser (KAM) techniques.

Interacting Systems

The analysis of noninteracting Fermi systems has been very successful in understanding qualitatively many features of crystals, but there are many properties (e.g., superconductivity or magnetism) which cannot be really explained without taking into account the interaction between fermions; however, the analysis becomes more involved. When there is no interaction, the properties of the many-body system can be understood in terms of the single-body properties; the eigenfunctions of the Hamiltonian are, in fact, obtained in terms of the single-particle eigenfunctions. This is not true when $\lambda \neq 0$ when a description of the system in terms of independent particles is impossible. In order to compute the interacting Schwinger functions, it is convenient to write them in terms of fermionic functional integrals (Berezin 1966). One introduces a set of anticommuting Grassmann variables $\psi_{\mathbf{k}}^+, \psi_{\mathbf{k}}^-$, $\mathbf{k} = (k_0, \mathbf{k})$; the Grassmann integration is defined by $\int d\psi_{\mathbf{k}}^\sigma \psi_{\mathbf{k}}^\sigma = 1$ and $\int d\psi_{\mathbf{k}}^\sigma = 0$, $\sigma = \pm$, and the integral of any analytic function of the Grassmann variables can be obtained by expanding it in Taylor series (which is a finite sum if suitable cutoffs are imposed and L, β are finite) and using the above rules; finally,

$$\psi_{\mathbf{x}}^+ = \frac{1}{L^d \beta} \sum_{\mathbf{k}} \phi_{\mathbf{k}}(\mathbf{x}) e^{ik_0 t} \psi_{\mathbf{k}}^+$$

and $\psi_{\mathbf{x}}^-$ is defined in an analogous way. The Schwinger function can be written as a Grassmann integral as follows:

$$S(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N) = \frac{\partial^N}{\partial \phi_{\mathbf{x}_1}^{\varepsilon_1} \dots \partial \phi_{\mathbf{x}_N}^{\varepsilon_N}} \log \int P(d\psi) e^{-\nu + \int d\mathbf{x} \phi_{\mathbf{x}}^{\varepsilon} \psi_{\mathbf{x}}^{\varepsilon}} \Big|_{\varphi=0} \quad [7]$$

where $P(d\psi)$ is the fermionic integration $[\prod_k d\psi_k^+ d\psi_k^-] \exp[\sum_k \psi_k^+ [-ik_0 + \varepsilon(\mathbf{k}) - \mu] \psi_k^-]$, while $\mathbf{y} = (\mathbf{y}, s)$, and

$$\nu = \lambda \sum_{\sigma, \sigma'} \int d\mathbf{x} d\mathbf{y} \nu(\mathbf{x} - \mathbf{y}) \times \delta(t - s) \psi_{x, \sigma}^+ \psi_{x, \sigma}^- \psi_{y, \sigma'}^+ \psi_{y, \sigma'}^- \quad [8]$$

The Grassmann integral of a monomial of Grassmann variables can be obtained by the Wick rule [5] with propagator the Fourier transform of $(-ik_0 + \varepsilon(\mathbf{k}) - \mu)^{-1}$. As stated earlier, the propagator is finite at nonzero temperature, whereas if $\beta = \infty$, then it is singular when $\mathbf{k} = (k_0, \mathbf{k})$ is such that $k_0 = 0$ and $\varepsilon(\mathbf{k}) = \mu$.

One can write [7] as a series by Taylor-expanding the exponential and using the Wick rule; each order of the expansion can be represented as a sum of Feynman diagrams, very similar to the ones appearing in quantum field theory. We have then an algorithm to compute [7]; nevertheless, to extract information from such a series is quite difficult. One cannot really compute an infinite (in the $L = \infty$ limit) number of coefficients, so one is tempted, for small λ , to compute only the first few of them, neglecting the others. However, it appears that this approximation is generally not justified, and it leads to wrong results; the reason is that the Schwinger functions for $\lambda = 0$ or $\lambda \neq 0$ are not analytically close, or, in more physical terms, even if λ is small, the physical behavior of the free and interacting theories can be quite different, especially at low temperatures. A number of very interesting concepts (e.g., spontaneous symmetry breaking or the mass generation phenomenon), or techniques (e.g., the renormalization group method, or the parquet or random phase approximation) have been introduced in the last 50 years to analyze [7], and indeed many results have been obtained which explain several physical properties of the matter, such as superconductivity or the Kondo effect (see, e.g., Anderson 1985, Abrikosov *et al.* 1965, Mahan 1990, Negele and Orland 1988, Pines 1961). Unfortunately, most of such results are not really mathematically consistent, and in many cases quantitative computations are impossible (in computations one generally neglects terms which, according to a heuristic physical intuition, are irrelevant, but no control of the error introduced by this approximation is attempted). In recent times, attempts towards a mathematical understanding of the functional integral [7] have started (see, e.g., Benfatto and Gallavotti (1995), and references therein); the methods rely on the mathematical implementation of Wilson's renormalization group methods via

multiscale analysis (Gallavotti 1985). The necessity of a firmer mathematical basis was felt mainly under the pressure of the recent discovery of high- T_c superconductors whose behavior is still not understood in terms of the microscopic model [7]; this has forced reconsideration of the validity of the approximations usually made in the analysis of this model.

The behavior of [7] depends crucially on the temperature. At high temperatures, we can simply expand the exponential in [7] in a power series of λ , and find that each Feynman graph contributing to the n th perturbative order is bounded by $C_\beta^n |\lambda|^n$, with $C_\beta \leq C\beta^\gamma$ for some constants C, γ ; this follows immediately by using the Wick rule and by remembering that the propagator is larger than $O(\beta^{-1})$. As the number of Feynman graphs contributing to order n is $O(n!)$, a bound on each Feynman graph is not sufficient to prove the convergence of the series. To prove convergence, one has to take into account cancellations, due to the anticommutativity of fermionic variables. Such cancellations are proved via Gram's inequality for determinants and a bound $C_\beta^n \lambda^n$ can be obtained for the order n (without factorials); hence, convergence follows for temperatures greater than $O(|\lambda|^\alpha)$ for some constant $\alpha > 0$. One finds that $S(\mathbf{k}) = S_0(\mathbf{k})(1 + A_\lambda(\mathbf{k}))$ with $|A_\lambda(\mathbf{k})| \leq C|\lambda|$, that is, the interaction has essentially no influence on the physical properties of the system at high temperatures.

Landau Fermi Liquids

We consider next an intermediate region of temperatures, that is, $e^{-a/|\lambda|} \leq T \leq |\lambda|^\alpha$ for some constants a, α . In this region, the naive expansion in power series of λ fails and other techniques, such as renormalization group, are necessary. Such a method allows us to perform a suitable resummation of the naive power series in λ , and one gets, for λ small enough, $T \geq e^{-a/|\lambda|}$ and $\varepsilon(\mathbf{k}) = |\mathbf{k}|^2/2m$,

$$\hat{S}(\mathbf{k}) = \frac{1}{Z(\lambda)} \frac{1 + A_\lambda(\mathbf{k})}{-ik_0 + \nu_F(\lambda)[|\mathbf{k}| - k_F(\lambda)]} \quad [9]$$

where $Z(\lambda) = 1 + z(\lambda)$, $\nu_F(\lambda) = \hbar k_F/m + \nu(\lambda)$, and $k_F(\lambda) = k_F + \nu(\lambda)$, with $z(\lambda) = O(\lambda^2)$, $\nu(\lambda) = O(\lambda)$, $\nu(\lambda) = O(\lambda^2)$, and $z(\lambda), \nu(\lambda), \nu_F(\lambda)$ essentially temperature independent; moreover, $|A_\lambda(\mathbf{k})|$ is $O(\lambda)$. The above formula has been proved rigorously for $d=2$ (see Rivasseau (1994), and references therein); for $d=3$, it has been proved at the level of formal perturbation theory (Benfatto and Gallavotti 1995). The case $\varepsilon(\mathbf{k}) = |\mathbf{k}|^2/2m$ is quite special, as the shape

of the interacting Fermi surface is fixed by the rotation-invariant symmetry; it is necessarily circular ($d=2$) or spherical ($d=3$), whereas in general the interaction can also modify its shape. For $d=2$, if the interacting Fermi surface is symmetric, smooth and convex, a formula like [9] still holds (with a function $k_F(\lambda, \mathbf{k})$ replacing $k_F(\lambda)$) up to exponentially small temperatures (see references in Gentile and Mastropietro (2001)).

It is apparent from [9] that one cannot derive such a formula from a power-series expansion in λ ; by expanding [9] as a series in λ , one immediately finds that the n th term is $O(\lambda^n \beta^n)$, which means that the naive perturbative expansion cannot be convergent up to exponentially small temperatures. It can be derived only by selecting and resumming some special class of terms in the original expansion. A peculiar property of [9] is that the wave function renormalization $Z(\lambda)$ is essentially independent of the temperature. Such temperature independence is a consequence of cancellations in the perturbative series essentially due to the curvature of the Fermi surface. For $d=1$, a formula similar to [9] is also valid; however, such cancellations are not present and one finds $Z(\lambda) = 1 + O(\lambda^2 \log \beta)$. Comparing $S(\mathbf{k})$ given by [9] with the Fourier transform $S_0(\mathbf{k})$ of [6], we note that the Schwinger function of the interacting system is still very similar to the Schwinger function of a free Fermi gas, with physical parameters (e.g., the Fermi momentum, the wave function renormalization, or the Fermi velocity) which are changed by the interaction. This property is quite remarkable: the eigenstates cannot be constructed when $\lambda=0$ starting from the single-particle states but, nevertheless, the physical properties of the interacting system (which can be deduced from the Schwinger functions) are qualitatively very similar to the ones of the free Fermi gas, although with different parameters; this explains why the free Fermi gas model works so well to explain the properties of crystals, although one neglects the interactions between fermions which are, of course, quite relevant. A fermionic system with such a property is called a Landau Fermi liquid (see, e.g., Arbiksov *et al.* 1965, Mahan 1990, Pines 1961), after Landau, who postulated in the 1950s that interacting systems may evolve continuously from the free system in many cases.

It was generally accepted that metals in this range of temperatures were all Landau Fermi liquids (except one-dimensional systems). However, the experimental discovery of the high- T_c superconductors (see, e.g., Anderson (1997)) has changed this belief, as such metals in their normal state, that is, above T_c are not Landau Fermi liquids; their

wave function renormalization behaves like $1 + O(\lambda^2 \log \beta)$ instead of $1 + O(\lambda^2)$ as in Landau Fermi liquid. This behavior has been called marginal-Fermi-liquid behavior and many attempts have been devoted to predict such behavior from [7]. In order to see deviations from Fermi liquid behavior, one could consider Fermi surfaces with flat or almost flat sides or corners (which are quite possible; e.g., in a square lattice with one conduction electron per atom, such as in the “half-filled Hubbard model”).

Let us finally consider the last regime, that is, temperatures lower than $O(e^{-a/|\lambda|})$. Except for very exceptional cases (e.g., asymmetric Fermi surfaces, i.e., such that $\varepsilon(\mathbf{k}) \neq \varepsilon(-\mathbf{k})$ except for a finite number of points, in which Fermi liquid behavior is found down to $T=0$ (Feldman *et al.* 2002)), a strong deviation from Fermi liquid behavior is observed; the interacting Schwinger function is not similar to the free one and the physical properties in this regime are totally new.

One-Dimensional Systems up to $T=0$

The only case in which the Schwinger functions of the Hamiltonian [3] can be really computed down to $T=0$ occurs for $d=1$; in such a case, an expression like [9] is not valid anymore and the system is not a Fermi liquid. On the contrary, when $u=0$ and for small repulsive $\lambda > 0$, one can prove, for spinning fermions (see Benfatto and Gallavotti (1995), Gentile and Mastropietro (2001) and references therein) that

$$\hat{S}(\mathbf{k}) = \frac{[k_0^2 + v_F^2(\lambda)(|\mathbf{k}| - k_F(\lambda))^2]^{\eta(\lambda)}}{-ik_0 + v_F(\lambda)[|\mathbf{k}| - k_F(\lambda)]} [1 + A_\lambda(\mathbf{k})] \quad [10]$$

where $k_F(\lambda) = k_F + O(\lambda)$ and $\eta(\lambda) = a\lambda^2 + O(\lambda^3)$ is a critical index. This means that the interaction changes qualitatively the nature of the singularity at the Fermi surface; $S(\mathbf{k})$ is still diverging at the Fermi surface but with an exponent which is no longer 1 but is $1 - 2\eta(\lambda)$, with $\eta(\lambda)$ a nonuniversal (i.e., λ -dependent) critical index. As a consequence, the physical properties are different with respect to the free Fermi gas; for instance, the occupation number $n_{\mathbf{k}}$ is not discontinuous at $k = \pm k_F(\lambda)$ when $T=0$. Nonuniversal critical indices appear in all the other response functions. Fermionic systems behaving in this way are called Luttinger liquids, as they behave like the exactly solvable Luttinger model describing relativistic spinless fermions with linear dispersion relation. The solvability of this model, due to Mattis and Lieb (1966), relies

on the possibility of mapping its Hamiltonian in a system of free bosons. Such a mapping is not possible for the Hamiltonian [3], which is not solvable; however, one can use renormalization group methods and suitable Ward identities to show that its behavior is similar to the Luttinger model (in a sense, one makes perturbation theory not around the free Fermi gas, but around the Luttinger model).

If we take into account the interaction with an external periodic potential with period a , that is, consider $u \neq 0$, we find that if $k_F \neq n\pi/a$, then the Schwinger function behaves essentially like [8]. On the contrary, in the filled-band case, $k_F = n\pi/a$, one finds that there is still an energy gap which becomes $O(u^{1+\eta})$ with $\eta_1 = O(\lambda)$; this means that the renormalization of the gap is described by a critical index; moreover, $S(x) \simeq O(e^{-|u|^{1+\eta}|x|})$. A similar behavior is also observed in the presence of quasi-periodic potential. In the attractive case, $\lambda < 0$, $u = 0$, the behavior is much less understood; it is believed that the interaction produces a gap Δ_λ in the spectrum which is nonanalytic in λ , and $S(x)$ shows an exponential decay rather than a power-law decay, and the interaction converts the system from a metal to an insulator.

Finally, it is remarkable that a large variety of models, like Heisenberg spin chains or bidimensional classical statistical mechanics models, such as the eight-vertex or the Ashkin–Teller model, can be mapped into interacting $d = 1$ fermionic systems, and consequently their critical behavior can be understood by using fermionic techniques (see Gentile and Mastropietro (2001), and references therein).

Superconductors

The theory up to $T = 0$ for $d = 2, 3$ systems with dispersion relation $|k|^2/2m$ is based only on approximate computations, predicting the phenomenon of superconductivity. According to the theory of Bardeen, Cooper, and Schrieffer (BCS theory), the interaction between fermions leads to the formation of a gap in the energy spectrum, below the critical temperature. There are many ways to derive the BCS theory. One is based on the fact that one verifies, by perturbative computations, that the effective interaction is stronger when the four momenta of the fermions are such that $k_1 \simeq -k_3$ and $k_2 \simeq -k_4$. This suggests, heuristically, to replace in [7] ν with

$$\nu_{\text{BCS}} = -\lambda \frac{1}{\beta L^{3d}} \sum_{k, k'} \psi_{k, \sigma}^+ \psi_{-k, -\sigma}^+ \psi_{k', -\sigma'}^- \psi_{-k', \sigma'}^-$$

which is an interaction between pairs of electrons with opposite spin and momenta, which are called Cooper pairs. Replacing ν with ν_{BCS} has the great advantage that it makes the Schwinger functions exactly computable and explains the mechanism of superconductivity in many metals (but not in the recently discovered high- T_c superconductors). On the other hand, proving that [7] with ν or ν_{BCS} has a similar behavior is still an important open problem. The two-point Schwinger function in the model with ν_{BCS} can be written, after the so-called Hubbard–Stratonovitch transformation, as

$$\hat{S}(k_0, k) = -\beta L^d \frac{\int \frac{-ik_0 - \varepsilon(k) + \mu}{k_0^2 + \varepsilon^2(k) + \lambda u^2} e^{-\beta L^d \nu(u)} du}{\int e^{-\beta L^d \nu(u)} du} \quad [11]$$

where $\nu(u)$ is a function with a global minimum in $u = 0$ for repulsive interactions $\lambda < 0$, whereas for $\lambda > 0$ and sufficiently small temperatures (for $T \leq T_c$, with $T_c = O(e^{-a/|\lambda|})$), it has the form of a double well with two minima at $u = \pm \Delta_\lambda$ with $\Delta_\lambda = O(e^{-a/|\lambda|})$; for T greater than T_c , there is only a global minimum at $u = 0$. By the saddle-point theorem, we find, for $T \leq T_c$ and $\lambda < 0$,

$$\lim_{L \rightarrow \infty} S(k) = \frac{-ik_0 - \varepsilon(k) + \mu}{k_0^2 + (\varepsilon(k) - \mu)^2 + \Delta_\lambda^2} \quad [12]$$

The physical properties predicted by [12] are completely different with respect to the free case: the occupation number is continuous, there is an energy gap in the spectrum, the specific heat is $O(e^{-\Delta_\lambda/T})$ and the phenomenon of superconductivity appears. The fact that the interaction generates a gap is called mass generation; a similar mechanism appears in particle theory.

Conclusions

Many other physical phenomena, observed experimentally, can be essentially understood by studying fermionic systems, but a clear mathematical comprehension is still lacking. We mention: the Kondo effect, that is, the resistance minimum observed in some metals due to magnetic impurities; Mott transition, in which a strong interaction produces an insulating state in a system which should be conductors; antiferromagnetism; fractional quantum Hall effect, and many others. We can say that the situation in this area of study reminds one of the classical mechanics at the end of the nineteenth century; there is agreement on the models to consider, which are believed to be able to take into

account the marvelous properties of the matter experimentally found, but to extract information from them requires deeper and complex analytical and mathematical investigations.

See also: Falicov–Kimball Model; Fractional Quantum Hall Effect; Quantum Statistical Mechanics: Overview; Renormalization: Statistical Mechanics and Condensed Matter.

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Feynman Path Integrals

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Introduction

In nonrelativistic quantum mechanics, the state of a d -dimensional particle is represented by a unitary vector ψ in the complex separable Hilbert space $L^2(\mathbb{R}^d)$, the so-called “wave function,” while its time evolution is described by the Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} \psi = -\frac{\hbar^2}{2m} \Delta \psi + V\psi \quad [1]$$

$$\psi(0, x) = \psi_0(x)$$

where \hbar is the reduced Planck constant, $m > 0$ is the mass of the particle, and $F = -\nabla V$ is an external force.

In 1942 R P Feynman, following a suggestion by Dirac, proposed an alternative (Lagrangian) formulation of quantum mechanics, and a heuristic but very suggestive representation for the solution of eqn [1]. According to Feynman, the wave function of the system at time t evaluated at the point $x \in \mathbb{R}^d$ is given as an “integral over histories,” or as an integral over all possible paths γ in the configuration

space of the system with finite energy passing at the point x at time t :

$$\psi(t, x) = \left(\int_{\{\gamma | \gamma(t) = x\}} e^{(i/\hbar) S_t^\circ(\gamma)} D\gamma \right)^{-1} \times \int_{\{\gamma | \gamma(t) = x\}} e^{(i/\hbar) S_t(\gamma)} \psi_0(\gamma(0)) D\gamma \quad [2]$$

$S_t(\gamma)$ is the classical action of the system evaluated along the path γ

$$S_t(\gamma) \equiv S_t^\circ(\gamma) - \int_0^t V(\gamma(s)) ds \quad [3]$$

$$S_t^\circ(\gamma) \equiv \frac{m}{2} \int_0^t |\dot{\gamma}(s)|^2 ds \quad [4]$$

$D\gamma$ is a heuristic Lebesgue “flat” measure on the space of paths and $(\int_{\{\gamma | \gamma(t) = x\}} e^{(i/\hbar) S_t^\circ(\gamma)} D\gamma)^{-1}$ is a normalization constant.

Some time later, Feynman himself extended formula [2] to more general quantum systems, including the case of quantum fields.

The Feynman path-integral formulation of quantum mechanics is particularly suggestive, as it provides a spacetime visualization of quantum dynamics, reintroducing in quantum mechanics the concept of trajectory (which was banned in the “orthodox interpretation” of the theory) and creating a connection between the classical description of

the physical world and the quantum one. Indeed, it provides a quantization method, allowing, at least heuristically, to associate a quantum evolution to each classical Lagrangian. Moreover, the application of the stationary-phase method for oscillatory integrals allows the study of the semiclassical limit of the Schrödinger equation, that is, the study of the detailed behavior of the solution when the Planck constant is regarded as a parameter converging to 0. Indeed, when \hbar is small, the integrand in [2] is strongly oscillating and the main contributions to the integral should come from those paths γ that make stationary the phase function $S(\gamma)$. These, by Hamilton's least action principle, are exactly the classical orbits of the system.

Feynman path integrals allow also a heuristic calculus in path space, leading to variational calculations of quantities of physical and mathematical interest. An interesting application can be found in topological field theories, as, for instance, Chern–Simons models. In this case, heuristic calculations based on the Feynman path-integral formulation of the theory, where the integration is performed on a space of geometrical objects, lead to the computation of topological invariants.

Even if from a physical point of view, formula [2] is a source of important results, from a mathematical point of view, it lacks rigor: indeed, neither the “infinite-dimensional Lebesgue measure,” nor the normalization constant in front of the integral is well defined. In this article, we shall describe the main approaches to the rigorous mathematical realization of Feynman path integrals, as well as their most important applications.

Possible Mathematical Definitions of Feynman's Measure

In the rigorous mathematical definition of Feynman's complex measure

$$\mu_F := \left(\int_{\{\gamma | \gamma(t)=x\}} e^{(i/\hbar)S_t^o(\gamma)} D\gamma \right)^{-1} e^{(i/\hbar)S_t^o(\gamma)} D\gamma \quad [5]$$

one has to face mainly two problems. First of all, the integral is defined on a space of paths, that is, on an infinite-dimensional space. The implementation of an integration theory is nontrivial: for instance, it is well known that a Lebesgue-type measure cannot be defined on infinite-dimensional Hilbert spaces. Indeed, the assumption of the existence of a σ -additive measure μ which is invariant under rotations and translations and assigns a positive finite measure to all bounded open sets leads to a

contradiction. In fact, by taking an orthonormal system $\{e_i\}_{i \in \mathbb{N}}$ in an infinite-dimensional Hilbert space \mathcal{H} and by considering the open balls $B_i = \{x \in \mathcal{H}, \|x - e_i\| < 1/2\}$, one has that they are pairwise disjoint and their union is contained in the open ball $B(0, 2) = \{x \in \mathcal{H}, \|x\| < 2\}$. By the Euclidean invariance of the Lebesgue-type measure μ , one can deduce that $\mu(B_i) = a$, $0 < a < \infty$, for all $i \in \mathbb{N}$. By the σ -additivity, one has

$$\mu(B(0, 2)) \geq \mu(\cup_i B_i) = \sum_i \mu(B_i) = \infty$$

but, on the other hand, $\mu(B(0, 2))$ should be finite as $B(0, 2)$ is bounded. As a consequence, we can also deduce that the term $D\gamma$ in [2] does not make sense.

The second problem is the fact that the exponent in the density $e^{(i/\hbar)S_t^o(\gamma)}$ is imaginary, so that the exponential oscillates. Even in finite dimensions, integrals of the form $\int_{\mathbb{R}^N} e^{i\Phi(x)} f(x) dx$, with $\Phi, f: \mathbb{R}^N \rightarrow \mathbb{R}$ are continuous functions and f is not summable, have to be suitably defined, in order to exploit the cancelations in the integral due to the oscillatory behavior of the exponential.

The study of the rigorous foundation of Feynman path integrals began in the 1960s, when Cameron proved that Feynman's heuristic complex measure [5] cannot be realized as a complex bounded variation σ -additive measure, even on very nice subsets of the space $(\mathbb{R}^d)^{[0, t]}$ of paths, contrary to the case of complex measures on \mathbb{R}^n of the form $e^{(i/2)|x|^2} dx$. In other words, it is not possible to implement an integration theory in the traditional (Lebesgue) sense. As a consequence, mathematicians tried to realize [5] as a linear continuous functional on a sufficiently rich Banach algebra of functions, inspired by the fact that a bounded measure can be regarded as a continuous functional on the space of bounded continuous functions. In order to mirror the features of the heuristic Feynman's measure, such a functional should have some properties:

1. it should behave in a simple way under “translations and rotations in path space,” as $D\gamma$ denotes a “flat” measure;
2. it should satisfy a Fubini-type theorem, concerning iterated integrations in path space (allowing the construction, in physical applications, of a one-parameter group of unitary operators);
3. it should be approximable by finite-dimensional oscillatory integrals, allowing a sequential approach in the spirit of Feynman's original work; and
4. it should be sufficiently flexible to allow a rigorous mathematical implementation of an infinite-dimensional version of the stationary-phase

method and the corresponding study of the semiclassical limit of quantum mechanics.

Nowadays, several implementations of this program can be found in the literature of physics and mathematics, for instance, by means of analytic continuation of Wiener integrals, or as an infinite-dimensional distribution in the framework of Hida calculus, or via "complex Poisson measures," or via nonstandard analysis, or as an infinite-dimensional oscillatory integral. The last of these methods is particularly interesting as it allows the systematic implementation of an infinite-dimensional version of the stationary-phase method, which can be applied to the study of the semiclassical limit of the solution of the Schrödinger equation [1].

Analytic Continuation

In one of the first approaches in the definition of Feynman path integrals, formula [2] was realized as the analytic continuation in a suitable complex parameter of a (nonoscillatory) Gaussian integral on the space of paths.

In 1949, inspired by Feynman's work, M Kac observed that by considering the heat equation

$$\begin{aligned} -\frac{\partial}{\partial t}u &= -\frac{1}{2m}\Delta u + V(x)u \\ u(0, x) &= \psi_0(x) \end{aligned} \quad [6]$$

instead of the Schrödinger equation [1] and by replacing the oscillatory term $e^{(i/\hbar)S_0(\gamma)}$ in Feynman complex measure with the fast decreasing one $e^{-(1/\hbar)S_0(\gamma)}$, it is possible to give a well-defined mathematical meaning to Feynman's heuristic formula [2] in terms of a well-defined integral on the space of continuous paths $W_{t,x} = \{w \in C(0, t; \mathbb{R}^d) : w(0) = x\}$ with respect to the Wiener Gaussian measure $P_{t,x}$:

$$\begin{aligned} u(t, x) &= \int_{W_{t,x}} e^{-\int_0^t V(\sqrt{1/m}w(\tau))d\tau} \\ &\times \psi_0(\sqrt{1/m}w(t)) dP_{t,x}(w) \end{aligned} \quad [7]$$

The path-integral representation [7] for the solution of the heat equation [6] is called Feynman-Kac formula.

The underlying idea of the analytic continuation approach comes from the fact that by introducing in [6] a suitable parameter λ , proportional, for instance, to the time t as in the case $\lambda = \lambda_1$,

$$\begin{aligned} -\lambda_1 \hbar \frac{\partial}{\partial t}u &= -\frac{1}{2m}\hbar^2 \Delta u + V(x)u \\ u(t, x) &= \int_{W_{t,x}} e^{-(1/\lambda_1 \hbar) \int_0^t V(\sqrt{\hbar/(m\lambda_1)}w(\tau))d\tau} \\ &\times \psi_0\left(\sqrt{\hbar/(m\lambda_1)}w(t)\right) dP_{t,x}(w) \end{aligned}$$

or to the Planck constant, as in the case $\lambda = \lambda_2$,

$$\begin{aligned} \lambda_2 \frac{\partial}{\partial t}u &= \frac{1}{2m}\lambda_2^2 \Delta u + V(x)u \\ u(t, x) &= \int_{W_{t,x}} e^{(1/\lambda_2) \int_0^t V(\sqrt{\lambda_2/m}w(\tau))d\tau} \\ &\times \psi_0(\sqrt{\lambda_2/m}w(t)) dP_{t,x}(w) \end{aligned}$$

or to the mass, as in the case $\lambda = \lambda_3$,

$$\begin{aligned} \frac{\partial}{\partial t}u &= \frac{1}{2\lambda_3}\Delta u - iV(x)u \\ u(t, x) &= \int_{W_{t,x}} e^{-i \int_0^t V(\sqrt{1/\lambda_3}w(\tau))d\tau} \\ &\times \psi_0(\sqrt{1/\lambda_3}w(t)) dP_{t,x}(w) \end{aligned}$$

and by allowing λ to assume complex values, then one gets, at least heuristically, Schrödinger equation and its solution by substituting, respectively, $\lambda_1 = -i$, $\lambda_2 = i\hbar$, or $\lambda_3 = -im$. These procedures can be made completely rigorous under suitable conditions on the potential V and initial datum ψ_0 .

The Approach via Fourier Transform

This approach has its roots in a couple of papers by K Ito in the 1960s and was extensively developed by S Albeverio and R Høegh-Krohn in the 1970s. The main idea is the definition of oscillatory integrals with quadratic phase function on a real separable Hilbert space $(\mathcal{H}, \langle \cdot, \cdot \rangle)$, the Fresnel integrals,

$$\widetilde{\int}_{\mathcal{H}} e^{(i/2\hbar)\|x\|^2} f(x) dx \quad [8]$$

as the distributional pairing between $e^{(i/2\hbar)\|x\|^2}$ and a complex-valued function f belonging to the space $\mathcal{F}(\mathcal{H})$ of functions that are Fourier transforms of complex bounded variation measures on \mathcal{H} , that is,

$$f = \hat{\mu}_f, \quad f(x) = \int_{\mathcal{H}} e^{i\langle x, y \rangle} d\mu_f(y)$$

$\mathcal{F}(\mathcal{H})$ is a Banach algebra, where the product is the pointwise one and the identity is the function $f(x) = 1 \forall x \in \mathcal{H}$. The norm of an element f is the total variation of the corresponding measure μ_f , that is, $\|\mu_f\| = \sup \sum_i |\mu_f(E_i)|$, where the supremum is taken over all sequences $\{E_i\}$ of pairwise-disjoint Borel subsets of \mathcal{H} , such that $\cup_i E_i = \mathcal{H}$.

Given a function $f \in \mathcal{F}(\mathcal{H})$, $f = \hat{\mu}_f$, its Fresnel integral is defined by the Parseval formula:

$$\widetilde{\int}_{\mathcal{H}} e^{(i/2\hbar)\|x\|^2} f(x) dx := \int_{\mathcal{H}} e^{-(i\hbar/2)\|x\|^2} d\mu_f(x) \quad [9]$$

where the right-hand side is a well-defined absolutely convergent integral with respect to a σ -additive measure on \mathcal{H} .

It is important to recall that this approach provides the implementation of a method of stationary phase for the expansion of the integral in powers of the small parameter \hbar occurring in the integrand. We postpone the discussion of these results, as well as the application to the solution of the Schrödinger equation, to the next section where a generalization of the present approach is described.

Infinite-Dimensional Oscillatory Integrals

The main idea of this approach is the extension of the definition of oscillatory integrals with quadratic phase function [8] to infinite-dimensional Hilbert spaces by means of a twofold limiting procedure.

The study of integrals of the form

$$I(\hbar) := \int_{\mathbb{R}^N} e^{(i/\hbar)\Phi(x)} f(x) dx \quad [10]$$

where $\Phi(x): \mathbb{R}^N \rightarrow \mathbb{R}$ is the phase function and $f: \mathbb{R}^N \rightarrow \mathbb{C}$ a complex-valued continuous function, is a classical topic, largely developed in connection with various problems in mathematics (such as the theory of pseudodifferential operators) and physics (such as optics). Particular effort has been devoted to the study of the detailed behavior of the above integral in the limit of “strong oscillations,” that is, when $\hbar \rightarrow 0$, by means of the method of stationary phase.

Thanks to the cancellations due to the oscillatory term $e^{(i/2\hbar)\Phi(x)}$, the integral can still be defined, even if the function f is not summable, as the limit of a sequence of regularized, hence absolutely convergent, integrals. According to a Hörmander’s proposal, the oscillatory integral of a function $f: \mathbb{R}^N \rightarrow \mathbb{C}$ is well defined if, for each test function $\phi \in \mathcal{S}(\mathbb{R}^N)$, such that $\phi(0) = 1$, the limit

$$\lim_{\epsilon \rightarrow 0} \int_{\mathbb{R}^N} e^{(i/2\hbar)\Phi(x)} \phi(\epsilon x) f(x) dx$$

exists and is independent of ϕ .

This definition has been generalized in the 1980s by D Elworthy and A Truman to the case where the underlying space \mathbb{R}^N is replaced by a real separable infinite-dimensional Hilbert space $(\mathcal{H}, \langle \cdot, \cdot \rangle)$, under the assumption that the phase function is quadratic, that is, $\Phi(x) = \|x\|^2/2$. The “infinite-dimensional oscillatory integral”

$$\int_{\mathcal{H}} e^{(i/2\hbar)\|x\|^2} f(x) dx$$

is defined as the limit of a sequence of finite-dimensional approximations. More precisely, a function $f: \mathcal{H} \rightarrow \mathbb{C}$ is “integrable” if, for each increasing sequence $\{P_n\}_{n \in \mathbb{N}}$ of finite-dimensional projector operators in \mathcal{H} converging strongly to the identity operator as $n \rightarrow \infty$, the limit

$$\lim_{n \rightarrow \infty} \left(\int_{P_n \mathcal{H}} e^{(i/2\hbar)\|P_n x\|^2} dP_n x \right)^{-1} \times \int_{P_n \mathcal{H}} e^{(i/2\hbar)\|P_n x\|^2} f(P_n x) dP_n x \quad [11]$$

exists and is independent of the sequence $\{P_n\}_{n \in \mathbb{N}}$. In this case, the limit is denoted by

$$\int_{\mathcal{H}} e^{(i/2\hbar)\|x\|^2} f(x) dx$$

The description of the largest class of integrable functions is still an open problem, even in finite dimension, but it is possible to find some interesting subsets of it. In particular, any function belonging to $\mathcal{F}(\mathcal{H})$, the Banach algebra considered in the approach by Fourier transform, is integrable. Indeed, by assuming that the function f in [11] is of the type

$$f(x) = e^{-(i/\hbar)\langle x, Lx \rangle} g(x)$$

where $L: \mathcal{H} \rightarrow \mathcal{H}$ is a linear self-adjoint trace-class operator on \mathcal{H} such that $(I - L)$ is invertible and $g \in \mathcal{F}(\mathcal{H})$, that is, $g(x) = \int_{\mathcal{H}} e^{\langle x, y \rangle} d\mu_g(y)$, then it is possible to prove that f is integrable in the sense of definition [11] and the corresponding infinite-dimensional oscillatory integral can be explicitly computed in terms of a well-defined integral with respect to a bounded variation measure μ_f by means of the following Parseval’s type equality:

$$\begin{aligned} & \int_{\mathcal{H}} e^{(i/2\hbar)\|x\|^2} e^{-(i/\hbar)\langle x, Lx \rangle} g(x) dx \\ &= \det(I - L)^{-1/2} \int_{\mathcal{H}} e^{-(i\hbar/2)\langle x, (I - L)^{-1}x \rangle} d\mu_f(x) \end{aligned} \quad [12]$$

$\det(I - L)$ being the Fredholm determinant of the operator $I - L$, that is, the product of its eigenvalues, counted with their multiplicity. If $L = 0$, then we obtain eqn [9], so that we can look at the infinite-dimensional oscillatory integrals approach as a generalization of the Fourier transform approach, since it allows at least in principle to integrate a class of function larger than $\mathcal{F}(\mathcal{H})$. In fact, recently this feature has been used by S Alberverio and S Mazzucchi in the proof of a Parseval’s type equality similar to [12] for infinite-dimensional oscillatory integrals with polynomially growing phase functions.

Feynman’s heuristic formula [2] for the representation of the solution of the Schrödinger equation [1] can

be realized as an infinite-dimensional oscillatory integral on the Hilbert space \mathcal{H}_t of absolutely continuous paths $\gamma: [0, t] \rightarrow \mathbb{R}^d$ with fixed endpoint $\gamma(t) = 0$ and finite kinetic energy $\int_0^t \dot{\gamma}^2(\tau) d\tau < \infty$, endowed with the inner product $\langle \gamma_1, \gamma_2 \rangle = \int_0^t \dot{\gamma}_1(\tau) \dot{\gamma}_2(\tau) d\tau$. One has to take an initial datum $\psi_0 \in L^2(\mathbb{R}^d)$ that is the Fourier transform of a complex bounded variation measure on \mathbb{R}^d , that is, $\psi_0(x) = \int_{\mathbb{R}^d} e^{ik \cdot x} d\mu_0(k)$. Moreover, one has to assume that the potential V in [1] is the sum of a harmonic oscillator part plus a bounded perturbation V_1 that is the Fourier transform of a complex bounded variation measure μ_v on \mathbb{R}^d :

$$V(x) = \frac{1}{2} x \Omega^2 x + V_1(x)$$

$$V_1(x) = \int_{\mathbb{R}^d} e^{ik \cdot x} d\mu_v(k)$$

(Ω^2 being a symmetric positive $d \times d$ matrix).

In this case, it is possible to prove that the linear operator L on \mathcal{H}_t defined by

$$(\gamma, L\gamma) \equiv \int_0^t \gamma(\tau) \Omega^2 \gamma(\tau) d\tau$$

is self-adjoint and trace class, and $(I - L)$ is invertible. Moreover, by considering the function $v: \mathcal{H}_t \rightarrow \mathbb{C}$

$$v(\gamma) \equiv \int_0^t V_1(\gamma(\tau) + x) d\tau$$

$$+ 2x \Omega^2 \int_0^t \gamma(\tau) d\tau, \quad \gamma \in \mathcal{H}_t$$

it is possible to prove that the function $f: \mathcal{H}_t \rightarrow \mathbb{C}$ given by

$$f(\gamma) = e^{-(i/\hbar)v(\gamma)} \psi_0(\gamma(0) + x)$$

is the Fourier transform of a complex bounded variation measure μ_f on \mathcal{H}_t and the infinite-dimensional Fresnel integral of the function $g(\gamma) = e^{-(i/2\hbar)(\gamma, L\gamma)} f(\gamma)$, that is:

$$\int_{\gamma(t)=0} e^{(i/2\hbar) \int_0^t \dot{\gamma}^2(\tau) d\tau} e^{-(i/\hbar) \int_0^t V(\gamma(\tau)+x) d\tau} \psi_0(\gamma(0) + x) d\gamma$$

$$= \int_{\mathcal{H}_t} e^{(i/2\hbar)(\gamma, (I-L)\gamma)} e^{-(i/\hbar)v(\gamma)} \psi_0(\gamma(0) + x) d\mu_f(\gamma) \quad [13]$$

is well defined and it is equal to

$$\det(I - L)^{-1/2} \int_{\mathcal{H}_t} e^{-(i\hbar/2)(\gamma, (I-L)^{-1}\gamma)} d\mu_f(\gamma)$$

Moreover, it is a representation of the solution of equation [1] evaluated at $x \in \mathbb{R}^d$ at time t . Recently, solutions of the Schrödinger equation with quartic anharmonic potential via infinite-dimensional oscillatory integrals have been provided by S Albeverio and S Mazzucchi using a combination of Parseval formula and a new analytic method (the inclusion of

such potentials had been a stumbling block for many years).

In this framework, it is possible to implement an infinite-dimensional version of the stationary-phase method and study the asymptotic behavior of the oscillatory integrals in the limit $\hbar \rightarrow 0$.

The method of stationary phase was originally proposed by Stokes, who noted that when $\hbar \rightarrow 0$ the oscillatory integral [10] is $O(\hbar^n)$ for any $n \in \mathbb{N}$, provided that there are no critical points of the phase function Φ in the support of the function f . As a consequence, one can deduce that the leading contribution to the integral [10] should come from a neighborhood of those points $c \in \mathbb{R}^N$, such that $\nabla \Phi(c) = 0$. More precisely, by assuming that the set C of critical points is finite, that is, $C = \{c_1, \dots, c_k\}$ and that every critical point is nondegenerate, that is, $\det D^2 \Phi(c_i) \neq 0 \forall c_i \in C$, then one has

$$I(\hbar) \sim \sum_{c_i \in C} e^{(i/\hbar)\Phi(c_i)} I_i^*(\hbar) \quad [14]$$

where $I_i^*: \mathbb{R} \rightarrow \mathbb{C}$ are C^∞ functions of \mathbb{R} , such that

$$I_i^*(0) = f(c_i) (2\pi i \hbar)^{N/2} (\det D^2 \Phi(c_i))^{-1/2}$$

If some critical point is degenerate, the situation is more complicated: one has to take into account the type of degeneracy and apply the theory of unfoldings of singularities.

These results can be generalized to infinite-dimensional oscillatory integrals of the form

$$I(\hbar) = \int_{\mathcal{H}} e^{(i/2\hbar)(x, (I-L)x)} e^{-(i/\hbar)v(x)} g(x) dx \quad [15]$$

with $v(x) = \int_{\mathcal{H}} e^{i\langle x, y \rangle} d\mu(y)$, $g(x) = \int_{\mathcal{H}} e^{i\langle x, y \rangle} d\nu(y)$, μ, ν being complex bounded variation measures on \mathcal{H} satisfying suitable assumptions and $L: \mathcal{H} \rightarrow \mathcal{H}$ is a self-adjoint and trace-class linear operator, such that $(I - L)$ is invertible. Under suitable growth condition on the moments of the measures μ, ν and by assuming that the phase function $\Phi(x) = \langle x, (I - L)x \rangle - v(x)$ has a finite number of nondegenerate critical points c_1, \dots, c_s , it is possible to prove that the integral $I(\hbar)$ in [15] is equal to

$$I(\hbar) = \sum_{k=1}^s e^{(i/\hbar)\Phi(c_k)} I_k^*(\hbar) + I_0(\hbar)$$

for some C^∞ functions I_k^* satisfying:

$$I_k^*(0) = [\det(I - L - D^2 V(c_k))]^{-1/2} g(c_k)$$

$$k = 1, \dots, s$$

$$I_0^{(j)}(0) = 0, \quad j = 0, 1, 2, \dots$$

Moreover, under some additional smallness assumptions on v , it has been proved that the phase function Φ has a unique stationary point c and as $\hbar \rightarrow 0$

$$I(\hbar) \sim e^{(i/\hbar)\Phi(c)} I^*(\hbar)$$

for some C^∞ function I^* . Each term of the asymptotic expansion in powers of \hbar of the function I^* can be explicitly computed, and it is possible to prove that such an asymptotic expansion is Borel-summable and determines I^* uniquely.

The application of these results to the infinite-dimensional oscillatory integral representation [13] for the solution of the Schrödinger equation allows the study of its semiclassical limit. One has to consider a potential V that is the Fourier transform of a complex bounded variation measure μ on (\mathbb{R}^d) , such that $\int_{\mathbb{R}^d} e^{|\beta|\epsilon} d|\mu|(\beta) < \infty$ for some $\epsilon > 0$, and a particular form for the initial wave function $\psi_0(x) = e^{(i/\hbar)\phi(x)} \chi(x)$, where ϕ is real and $\phi, \chi \in C_0^\infty(\mathbb{R}^d)$ are independent of \hbar . This initial datum corresponds to an initial particle distribution $\rho_0(x) = |\chi|^2(x)$ and to a limiting value of the probability current $J_{\hbar=0} = \nabla\phi(x)\rho_0(x)/m$, giving an initial particle flux associated to the velocity field $\nabla\phi(x)/m$. One also has to assume that the Lagrange manifold $L_f \equiv (y, -\nabla f)$ intersects transversally the subset Λ_V of the phase space made of all points (y, p) such that p is the momentum at y of a classical particle that starts at time zero from x , moves under the action of V , and ends at y at time t . In this case, the Feynman path integral [13] has an asymptotic expansion in powers of \hbar for $\hbar \rightarrow 0$, whose leading term is the sum of the values of the function

$$\left| \det \left(\left(\frac{\partial \bar{\gamma}_k^{(j)}}{\partial y_l^{(j)}}(y^{(j)}, t) \right) \right) \right|^{-1/2} e^{-(i/2)\pi m^{(j)}} e^{-(i/\hbar)S} e^{-(i/\hbar)\phi} \chi$$

taken at the points $y^{(j)}$ such that a classical particle starting at $y^{(j)}$ at time zero with momentum $\nabla\phi(y^{(j)})$ is at x at time t . S is the classical action along this classical path $\bar{\gamma}^{(j)}$ and $m^{(j)}$ is the Maslov index of the path $\bar{\gamma}^{(j)}$, that is, $m^{(j)}$ is the number of zeros of

$$\det \left(\left(\frac{\partial \bar{\gamma}_k^{(j)}}{\partial y_l^{(j)}}(y^{(j)}, \tau) \right) \right)$$

as τ varies on the interval $(0, t)$.

White-Noise Calculus

The leading idea of the present approach, which was originally proposed by C DeWitt-Morette and P Krée and presently realized in the framework of white-noise calculus by T Hida, L Streit, and many other authors, is the realization of the Feynman

integrand $e^{(i/\hbar)S_t(\gamma)}$ as an infinite-dimensional distribution. This idea is similar to the one of the approach via Fourier transform, where the expression $(2\pi i)^{-d/2} \int_{\mathbb{R}^d} e^{(i/2)(x,x)} f(x) dx$ is realized as a distributional pairing between $e^{(i/2)(x,x)}/(2\pi i)^{d/2}$ and the function $f \in \mathcal{F}(\mathbb{R}^d)$ by means of the Parseval-type equality [9] and generalized to infinite-dimensional spaces. In white-noise calculus, the pairing is realized in a different measure space. Indeed, by manipulating the integrand in

$$(2\pi i)^{-d/2} \int_{\mathbb{R}^d} e^{(i/2)(x,x)} f(x) dx$$

one has

$$\begin{aligned} & \int_{\mathbb{R}^d} \frac{e^{(i/2)(x,x)}}{(2\pi i)^{d/2}} f(x) dx \\ &= \int_{\mathbb{R}^d} \frac{e^{(i/2)(x,x)+(1/2)(x,x)}}{i^{d/2}} f(x) \frac{e^{-(1/2)(x,x)}}{(2\pi)^{d/2}} dx \quad [16] \end{aligned}$$

where the latter line can be interpreted as the distributional pairing of

$$\frac{e^{(i/2)(x,x)+(1/2)(x,x)}}{i^{d/2}}$$

and f not with respect to Lebesgue measure but rather with respect to the standard Gaussian measure

$$\frac{e^{-(1/2)(x,x)}}{(2\pi)^{d/2}} dx$$

on \mathbb{R}^d . The RHS of [16] can be generalized to the case in which \mathbb{R}^d is replaced by a path space, thanks to the fact that on infinite-dimensional spaces, even if Lebesgue measure is meaningless, Gaussian measures are well defined and can be used as reference measures. The detailed realization of this idea as well as its application to the mathematical realization of the Feynman integrand are rather technical and we certainly do not provide details here. We recall that this approach has been successfully applied to the rigorous realization of Feynman path-integral formulation of Chern-Simons models.

Other Possible Approaches

Another possible mathematical definition of Feynman path integrals is based on Poisson measures. It was originally proposed by A M Chebotarev and V P Maslov and further developed by several authors such as S Albeverio, Ph Blanchard, Ph Combe, R Høegh-Krohn, M Sirugue, and V Kolokol'tsov. It can be applied to "phase-space integrals," to the Dirac equation and in particular algebraic settings, as well as to the Schrödinger

equation, with potentials of the same type “Fourier transform of bounded measure” discussed in the subsection “Infinite-dimensional oscillatory integrals.”

Another possible definition of Feynman path integrals is based on a “time-slicing” approximation and a limiting procedure, rather closed to Feynman’s original work based on Trotter product formula. The “sequential approach” was proposed originally by A Truman and further extensively developed by D Fujiwara and N Kumano-go. The paths γ in formula [2] are approximated by piecewise linear paths and the Feynman path integral is correspondingly approximated by a finite-dimensional integral. In particular, D Fujiwara and N Kumano-go proved that the integrals defined in this way have some important properties, such as invariance under translations and orthogonal transformations. It is also possible to interchange the order of integration with Riemann–Stieltjes integrals and study the semiclassical approximation.

Finally, it is worthwhile to recall a very interesting and intuitive approach to the Feynman integration which is based on nonstandard analysis. It was introduced by S Albeverio, J E Fenstad, R Høegh-Krohn, and T Linstrom in the 1980s, but it has not been systematically developed yet.

Abbreviations

$D\gamma$	Heuristic Lebesgue-type measure on the space of paths
$P_{t,x}$	Wiener Gaussian measure on $W_{t,x}$
S_t	Action functional
S_t°	Action functional for the free particle
V	Potential
$W_{t,x}$	Space of continuous paths with fixed initial point $W_{t,x} = \{w \in C(0, t; \mathbb{R}^d) : w(0) = x\}$
\hbar	Reduced Planck constant

Φ	Phase function
γ	Path, $\gamma : [0, t] \rightarrow \mathbb{R}^d$
$\hat{\mu}$	Fourier transform of the measure μ
ψ	Wave function, solution of the Schrödinger equation
\mathcal{H}	Hilbert space
$\int_{\mathcal{H}}$	Fresnel integral on the Hilbert space \mathcal{H}
$\int_{\mathcal{H}}^\circ$	Infinite-dimensional oscillatory integral on the Hilbert space \mathcal{H}
$\langle \cdot, \cdot \rangle$	inner product
$\ \cdot \ $	norm

See also: Chern–Simons Models: Rigorous Results; Euclidean Field Theory; Functional Integration in Quantum Physics; Path Integrals in Noncommutative Geometry; Quillen Determinant; Singularity and Bifurcation Theory; Stationary Phase Approximation.

Further Reading

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Finite-Dimensional Algebras and Quivers

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Introduction

Algebras and their representations are ubiquitous in mathematics. It turns out that representations of finite-dimensional algebras are intimately related to quivers, which are simply oriented graphs. Quivers

arise naturally in many areas of mathematics, including representation theory, algebraic and differential geometry, Kac–Moody algebras, and quantum groups. In this article, we give a brief overview of some of these topics. We start by giving the basic definitions of associative algebras and their representations. We then introduce quivers and their representation theory, mentioning the connection to the representation theory of associative algebras. We also discuss in some detail the relationship between quivers and the theory of Lie algebras.

Associative Algebras

An “algebra” is a vector space A over a field k equipped with a multiplication which is distributive and such that

$$a(xy) = (ax)y = x(ay), \quad \forall a \in k, x, y \in A$$

When we wish to make the field explicit, we call A a k -algebra. An algebra is “associative” if $(xy)z = x(yz)$ for all $x, y, z \in A$. A has a “unit,” or “multiplicative identity,” if it contains an element 1_A such that $1_A x = x 1_A = x$ for all $x \in A$. From now on, we will assume all algebras are associative with unit. A is said to be “commutative” if $xy = yx$ for all $x, y \in A$ and finite dimensional if the underlying vector space of A is finite dimensional.

A vector subspace I of A is called a “left (resp. right) ideal” if $xy \in I$ for all $x \in A, y \in I$ (resp. $x \in I, y \in A$). If I is both a right and a left ideal, it is called a two-sided ideal of A . If I is a two-sided ideal of A , then the factor space A/I is again an algebra.

An algebra homomorphism is a linear map $f: A_1 \rightarrow A_2$ between two algebras such that

$$f(1_{A_1}) = 1_{A_2}$$

$$f(xy) = f(x)f(y), \quad \forall x, y \in A$$

A representation of an algebra A is an algebra homomorphism $\rho: A \rightarrow \text{End}_k(V)$ for a k -vector space V . Here $\text{End}_k(V)$ is the space of endomorphisms of the vector space V with multiplication given by composition. Given a representation of an algebra A on a vector space V , we may view V as an A -module with the action of A on V given by

$$a \cdot v = \rho(a)v, \quad a \in A, v \in V$$

A morphism $\psi: V \rightarrow W$ of two A -modules (or equivalently, representations of A) is a linear map commuting with the action of A . That is, it is a linear map satisfying

$$a \cdot \psi(v) = \psi(a \cdot v), \quad \forall a \in A, v \in V$$

Let G be a commutative monoid (a set with an associative multiplication and a unit element). A G -graded k -algebra is a k -algebra which can be expressed as a direct sum $A = \bigoplus_{g \in G} A_g$ such that $aA_g \subset A_g$ for all $a \in k$ and $A_{g_1}A_{g_2} \subset A_{g_1+g_2}$ for all $g_1, g_2 \in G$. A morphism $\psi: A \rightarrow B$ of G -graded algebras is a k -algebra morphism respecting the grading, that is, satisfying $\psi(A_g) \subset B_g$ for all $g \in G$.

Quivers and Path Algebras

A “quiver” is simply an oriented graph. More precisely, a quiver is a pair $Q = (Q_0, Q_1)$ where Q_0 is a finite set of vertices and Q_1 is a finite set of arrows (oriented edges) between them. For $a \in Q_1$, we let $h(a)$ denote the “head” of a and $t(a)$ denote the “tail” of a . A path in Q is a sequence $x = \rho_1 \rho_2 \dots \rho_m$ of arrows such that $h(\rho_{i+1}) = t(\rho_i)$ for $1 \leq i \leq m-1$. We let $t(x) = t(\rho_m)$ and $h(x) = h(\rho_1)$ denote the initial and final vertices of the path x . For each vertex $i \in Q_0$, we let e_i denote the trivial path which starts and ends at the vertex i .

Fix a field k . The path algebra kQ associated to a quiver Q is the k -algebra whose underlying vector space has basis the set of paths in Q , and with the product of paths given by concatenation. Thus, if $x = \rho_1 \dots \rho_m$ and $y = \sigma_1 \dots \sigma_n$ are two paths, then $xy = \rho_1 \dots \rho_m \sigma_1 \dots \sigma_n$ if $h(y) = t(x)$ and $xy = 0$ otherwise. We also have

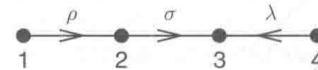
$$e_i e_j = \begin{cases} e_i & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

$$e_i x = \begin{cases} x & \text{if } h(x) = i \\ 0 & \text{if } h(x) \neq i \end{cases}$$

$$x e_i = \begin{cases} x & \text{if } t(x) = i \\ 0 & \text{if } t(x) \neq i \end{cases}$$

for $x \in kQ$. This multiplication is associative. Note that $e_i A$ and $A e_i$ have bases given by the set of paths ending and starting at i , respectively. The path algebra has a unit given by $\sum_{i \in Q_0} e_i$.

Example 1 Let Q be the following quiver:



then kQ has a basis given by the set of paths $\{e_1, e_2, e_3, e_4, \rho, \sigma, \lambda, \sigma\rho\}$. Some sample products are $\rho\sigma = 0, \lambda\lambda = 0, \lambda\sigma = 0, e_3\sigma = \sigma e_2 = \sigma, e_2\sigma = 0$.

Example 2 Let Q be the following quiver (the so-called “Jordan quiver”).



Then $kQ \cong k[t]$, the algebra of polynomials in one variable.

Note that the path algebra kQ is finite dimensional if and only if Q has no oriented cycles (paths with the same head and tail vertex).

Example 3 Let Q be the following quiver:



Then for every $1 \leq i \leq j \leq n$, there is a unique path from i to j . Let $f: kQ \rightarrow M_n(k)$ be the linear map from the path algebra to the $n \times n$ matrices with entries in the field k that sends the unique path from i to j to the matrix E_{ji} with (j, i) entry 1 and all other entries zero. Then one can show that f is an isomorphism onto the algebra of lower triangular matrices.

Representations of Quivers

Fix a field k . A representation of a quiver Q is an assignment of a vector space to each vertex and to each arrow a linear map between the vector spaces assigned to its tail and head. More precisely, a representation V of Q is a collection

$$\{V_i | i \in Q_0\}$$

of finite-dimensional k -vector spaces together with a collection

$$\{V_\rho: V_{t(\rho)} \rightarrow V_{h(\rho)} | \rho \in Q_1\}$$

of k -linear maps. Note that a representation V of a quiver Q is equivalent to a representation of the path algebra kQ . The dimension of V is the map $d_V: Q_0 \rightarrow \mathbb{Z}_{\geq 0}$ given by $d_V(i) = \dim V_i$ for $i \in Q_0$.

If V and W are two representations of a quiver Q , then a morphism $\psi: V \rightarrow W$ is a collection of k -linear maps

$$\{\psi_i: V_i \rightarrow W_i | i \in Q_0\}$$

such that

$$W_\rho \psi_{t(\rho)} = \psi_{h(\rho)} V_\rho, \quad \forall \rho \in Q_1$$

Proposition 1 Let A be a finite-dimensional k -algebra. Then the category of representations of A is equivalent to the category of representations of the algebra kQ/I for some quiver Q and some two-sided ideal I of kQ .

It is for this reason that the study of finite-dimensional associative algebras is intimately related to the study of quivers.

We define the direct sum $V \oplus W$ of two representations V and W of a quiver Q by

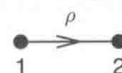
$$(V \oplus W)_i = V_i \oplus W_i, \quad i \in Q_0$$

and $(V \oplus W)_\rho: V_{t(\rho)} \oplus W_{t(\rho)} \rightarrow V_{h(\rho)} \oplus W_{h(\rho)}$ by

$$(V \oplus W)_\rho((v, w)) = (V_\rho(v), W_\rho(w))$$

for $v \in V_{t(\rho)}, w \in W_{t(\rho)}, \rho \in Q_1$. A representation V is “trivial” if $V_i = 0$ for all $i \in Q_0$ and “simple” if its only subrepresentations are the zero representation and V itself. We say that V is “decomposable” if it is isomorphic to $W \oplus U$ for some nontrivial representations W and U . Otherwise, we call V “indecomposable.” Every representation of a quiver has a decomposition into indecomposable representations that is unique up to isomorphism and permutation of the components. Thus, to classify all representations of a quiver, it suffices to classify the indecomposable representations.

Example 4 Let Q be the following quiver:



Then Q has three indecomposable representations U , V , and W given by:

$$\begin{array}{lll} U_1 = k, & U_2 = 0, & U_\rho = 0 \\ V_1 = 0, & V_2 = k, & V_\rho = 0 \\ W_1 = k, & W_2 = k, & W_\rho = 1 \end{array}$$

Then any representation Z of Q is isomorphic to

$$Z \cong U^{d_1-r} \oplus V^{d_2-r} \oplus W^r$$

where $d_1 = \dim Z_1, d_2 = \dim Z_2, r = \text{rank } Z_\rho$.

Example 5 Let Q be the Jordan quiver. Then representations V of Q are classified up to isomorphism by the Jordan normal form of V_ρ where ρ is the single arrow of the quiver. Indecomposable representations correspond to single Jordan blocks. These are parametrized by a discrete parameter n (the size of the block) and a continuous parameter λ (the eigenvalue of the block).

A quiver is said to be of “finite type” if it has only finitely many indecomposable representations (up to isomorphism). If a quiver has infinitely many isomorphism classes but they can be split into families, each parametrized by a single continuous parameter, then we say the quiver is of “tame” (or “affine”) type. If a quiver is of neither finite nor tame type, it is of “wild type.” It turns out that there is a rather remarkable relationship between the classification of quivers and their representations and the theory of Kac–Moody algebras.

The “Euler form” or “Ringel form” of a quiver Q is defined to be the asymmetric bilinear form on \mathbb{Z}^{Q_0} given by

$$\langle \alpha, \beta \rangle = \sum_{i \in Q_0} \alpha(i) \beta(i) - \sum_{\rho \in Q_1} \alpha(t(\rho)) \beta(h(\rho))$$

In the standard coordinate basis of \mathbb{Z}^{Q_0} , the Euler form is represented by the matrix $E = (a_{ij})$ where

$$a_{ij} = \delta_{ij} - \#\{\rho \in Q_1 \mid t(\rho) = i, h(\rho) = j\}$$

Here δ_{ij} is the Kronecker delta symbol. We define the “Cartan form” of the quiver Q to be the symmetric bilinear form given by

$$(\alpha, \beta) = \langle \alpha, \beta \rangle + \langle \beta, \alpha \rangle$$

Note that the Cartan form is independent of the orientation of the arrows in Q . In the standard coordinate basis of \mathbb{Z}^{Q_0} , the Cartan form is represented by the Cartan matrix $C = (c_{ij})$ where $c_{ij} = a_{ij} + a_{ji}$.

Example 6 For the quiver in Example 1, the Euler matrix is

$$E = \begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & 1 \end{pmatrix}$$

and the Cartan matrix is

$$C = \begin{pmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{pmatrix}$$

The “Tits form” q of a quiver Q is defined by

$$q(\alpha) = \langle \alpha, \alpha \rangle = \frac{1}{2}(\alpha, \alpha)$$

It is known that the number of continuous parameters describing representations of dimension α for $\alpha \neq 0$ is greater than or equal to $1 - q(\alpha)$.

Let \mathfrak{g} be the Kac–Moody algebra associated to the Cartan matrix of a quiver Q . By forgetting the orientation of the arrows of Q , we obtain the underlying (undirected) graph. This is the Dynkin graph of \mathfrak{g} . Associated to \mathfrak{g} is a root system and a set of simple roots $\{\alpha_i \mid i \in Q_0\}$ indexed by the vertices of the Dynkin graph.

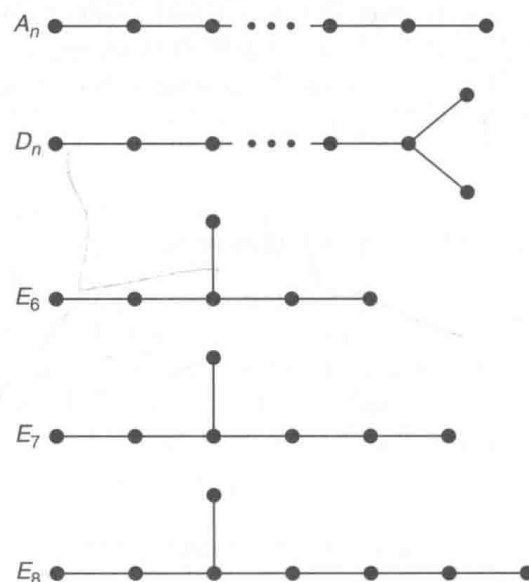
Theorem 1 (Gabriel’s theorem).

- (i) A quiver is of finite type if and only if the underlying graph is a union of Dynkin graphs of type A , D , or E .
- (ii) A quiver is of tame type if and only if the underlying graph is a union of Dynkin graphs of type A , D , or E and extended Dynkin graphs of type \hat{A} , \hat{D} , or \hat{E} (with at least one extended Dynkin graph).
- (iii) The isomorphism classes of indecomposable representations of a quiver Q of finite type are in one-to-one correspondence with the positive roots of the root system associated to the

underlying graph of Q . The correspondence is given by

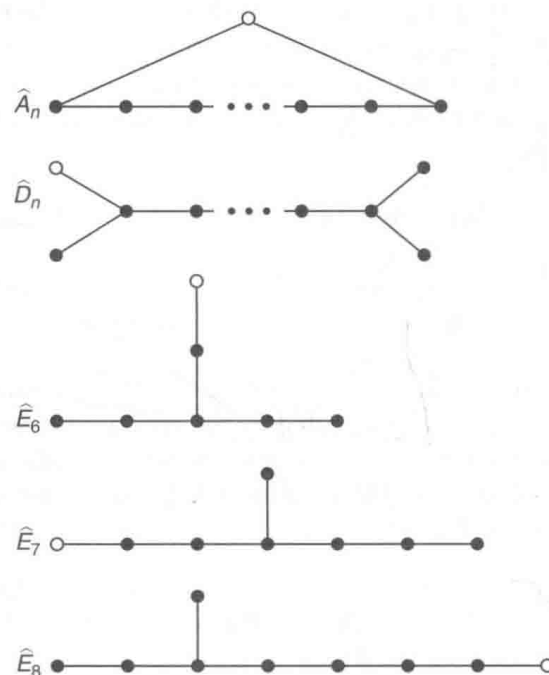
$$V \mapsto \sum_{i \in Q_0} d_V(i) \alpha_i$$

The Dynkin graphs of type A , D , and E are as follows.



Here the subscript indicates the number of vertices in the graph.

The extended Dynkin graphs of type \hat{A} , \hat{D} , and \hat{E} are as follows.



Here we have used an open dot to denote the vertex that was added to the corresponding Dynkin graph of type A , D , or E .

Theorem 2 (Kac’s theorem). Let Q be an arbitrary quiver. The dimension vectors of indecomposable representations of Q correspond to positive roots

of the root system associated to the underlying graph of Q (and are thus independent of the orientation of the arrows of Q). The correspondence is given by

$$d_V \mapsto \sum_{i \in Q_0} d_V(i) \alpha_i$$

Note that in Kac's Theorem, it is not asserted that the isomorphism classes are in one-to-one correspondence with the roots as in the finite case considered in Gabriel's theorem. It turns out that in the general case, dimension vectors for which there is exactly one isomorphism class correspond to real roots while imaginary roots correspond to dimension vectors for which there are families of representations.

Example 7 Let Q be the quiver of type A_n , oriented as follows.



It is known that the set of positive roots of the simple Lie algebra of type A_n is

$$\left\{ \sum_{i=j}^l \alpha_i \mid 1 \leq j \leq l \leq n \right\} \sqcup \{0\}$$

The zero root corresponds to the trivial representation. The root $\sum_{i=j}^l \alpha_i$ for some $1 \leq j \leq l \leq n$ corresponds to the unique (up to isomorphism) representation V with

$$V_i = \begin{cases} k & \text{if } j \leq i \leq l \\ 0 & \text{otherwise} \end{cases}$$

and

$$V_{\rho_i} = \begin{cases} 1 & \text{if } j \leq i \leq l-1 \\ 0 & \text{otherwise} \end{cases}$$

Example 8 Let Q be the quiver of type \hat{A}_n , with all arrows oriented in the same direction (for instance, counter-clockwise). The positive root $\sum_{i=0}^n \alpha_i$ (where $\{0, 1, 2, \dots, n\}$ are the vertices of the quiver) is imaginary. There is a one-parameter family of isomorphism classes of indecomposable representations where the maps assigned to each arrow are nonzero. The parameter is the composition of the maps around the loop.

If a quiver Q has no oriented cycles, then the only simple kQ -modules are the modules S^i for $i \in Q_0$ where

$$S_j^i = \begin{cases} k & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

and $S_\rho^i = 0$ for all $\rho \in Q_1$.

Ringel-Hall Algebras

Let k be the finite field \mathbb{F}_q with q elements and let Q be a quiver with no oriented cycles. Let \mathcal{P} be the set of all isomorphism classes of kQ -modules which are finite as sets (since k is finite dimensional, these are just the quiver representations we considered above). Let A be a commutative integral domain containing \mathbb{Z} and elements v, v^{-1} such that $v^2 = q$. The Ringel-Hall algebra $H = H_{A,v}(kQ)$ is the free A -module with basis $\{[V]\}$ indexed by the isomorphism classes of representations of the quiver Q , with an A -bilinear multiplication defined by

$$[V^1] \cdot [V^2] = v^{\langle \dim V^1, \dim V^2 \rangle} \sum_V g_{V^1, V^2}^V [V]$$

Here $\langle \dim V^1, \dim V^2 \rangle$ is the Euler form and g_{V^1, V^2}^V is the number of submodules W of V such that $V/W \cong V^1$ and $W \cong V^2$. H is an associative $\mathbb{Z}_{\geq 0}$ -graded algebra, with identity element $[0]$, the isomorphism class of the trivial representation. The grading $H = \bigoplus_\alpha H_\alpha$ is given by letting H_α be the A -span of the set of isomorphism classes $[V]$ such that $\dim V = \alpha$.

Let $C = C_{A,v}(kQ)$ be the A -subalgebra of H generated by the isomorphism classes $[S^i]$ of the simple kQ -modules. C is called the "composition algebra." If the underlying graph of Q is of finite type, then $C = H$.

Now let \mathcal{K} be a set of finite fields k such that the set $\{|k| \mid k \in \mathcal{K}\}$ is infinite. Let A be an integral domain containing \mathbb{Q} and, for each $k \in \mathcal{K}$, an element v_k such that $v_k^2 = |k|$. For each $k \in \mathcal{K}$, we have the corresponding composition algebra C_k , generated by the elements $[{}^k S^i]$ (here we make the field k explicit). Now let C be the subring of $\prod_{k \in \mathcal{K}} C_k$ generated by Q and the elements

$$\begin{aligned} t &= (t_k)_{k \in \mathcal{K}}, & t_k &= v_k \\ t^{-1} &= (t_k^{-1})_{k \in \mathcal{K}}, & t_k^{-1} &= (v_k)^{-1} \\ u^i &= (u_k^i)_{k \in \mathcal{K}}, & u_k^i &= [{}^k S^i], \quad i \in Q_0 \end{aligned}$$

Now, t lies in the center of C and if $p(t) = 0$ for some polynomial p , then p must be the zero polynomial since the set of v_k is infinite. Thus, we may think of C as the A -algebra generated by the $u^i, i \in Q_0$, with $A = \mathbb{Q}[t, t^{-1}]$ and t an indeterminate. Let $C^* = \mathbb{Q}(t) \otimes_A C$. We call C^* the "generic composition algebra."

Let \mathfrak{g} be the Kac-Moody algebra associated to the Cartan matrix of the quiver Q and let U be the quantum group associated by Drinfeld and Jimbo to \mathfrak{g} . It has a triangular decomposition $U = U^- \otimes U^0 \otimes U^+$.

Specifically, U^+ is the $\mathbb{Q}(t)$ -algebra with generators $E_i, i \in Q_0$ and relations

$$\sum_{p=0}^{1-c_{ij}} (-1)^p \begin{bmatrix} 1-c_{ij} \\ p \end{bmatrix} E_i^p E_j E_i^{1-c_{ij}-p}, \quad i \neq j$$

where c_{ij} are the entries of the Cartan matrix and

$$\begin{bmatrix} m \\ p \end{bmatrix} = \frac{[m]!}{[p]![m-p]!}$$

$$[n] = \frac{t^n - t^{-n}}{t - t^{-1}}, \quad [n]! = [1][2] \dots [n]$$

Theorem 3 *There is a $\mathbb{Q}(t)$ -algebra isomorphism $C^* \rightarrow U^+$ sending $u_i \mapsto E_i$ for all $i \in Q_0$.*

The proof of Theorem 3 is due to Ringel in the case that the underlying graph of Q is of finite or affine type. The more general case presented here is due to Green.

All of the Kac-Moody algebras considered so far have been simply-laced. That is, their Cartan matrices are symmetric. There is a way to deal with non-simply-laced Kac-Moody algebras using species. We will not treat this subject in this article.

Quiver Varieties

One can use varieties associated to quivers to yield a geometric realization of the upper half of the universal enveloping algebra of a Kac-Moody algebra \mathfrak{g} and its irreducible highest-weight representations.

Lusztig's Quiver Varieties

We first introduce the quiver varieties, first defined by Lusztig, which yield a geometric realization of the upper half U^+ of the universal enveloping algebra of a simply laced Kac-Moody algebra \mathfrak{g} . Let $Q = (Q_0, Q_1)$ be the quiver whose vertices Q_0 are the vertices of the Dynkin diagram of \mathfrak{g} and whose set of arrows Q_1 consists of all the edges of the Dynkin diagram with both orientations. By definition, U^+ is the \mathbb{Q} -algebra defined by generators $e_i, i \in Q_0$, subject to the Serre relations

$$\sum_{p=0}^{1-c_{ij}} (-1)^p \begin{bmatrix} 1-c_{ij} \\ p \end{bmatrix} e_i^p e_j e_i^{1-c_{ij}-p} = 0$$

for all $i \neq j$ in Q_0 , where c_{ij} are the entries of the Cartan matrix associated to Q . For any $\nu = \sum_{i \in Q_0} \nu_i i, \nu_i \in \mathbb{N}$, let U_ν^+ be the subspace of U^+ spanned by the

monomials $e_{i_1} e_{i_2} \dots e_{i_n}$ for various sequences i_1, i_2, \dots, i_n in which i appears ν_i times for each $i \in Q_0$. Thus, $U^+ = \bigoplus_\nu U_\nu^+$. Let U_Z^+ be the subring of U^+ generated by the elements $e_i^p / p!$ for $i \in Q_0, p \in \mathbb{N}$. Then $U_Z^+ = \bigoplus_\nu U_{Z,\nu}^+$ where $U_{Z,\nu}^+ = U_Z^+ \cap U_\nu^+$.

We define the involution $\bar{\cdot}: Q_1 \rightarrow Q_1$ to be the function which takes $\rho \in Q_1$ to the element of Q_1 consisting of the same edge with opposite orientation. An orientation of our graph/quiver is a choice of a subset $\Omega \subset Q_1$ such that $\Omega \cup \bar{\Omega} = Q_1$ and $\Omega \cap \bar{\Omega} = \emptyset$.

Let \mathcal{V} be the category of finite-dimensional Q_0 -graded vector spaces $V = \bigoplus_{i \in Q_0} V_i$ over \mathbb{C} with morphisms being linear maps respecting the grading. Then $V \in \mathcal{V}$ shall denote that V is an object of \mathcal{V} . The dimension of $V \in \mathcal{V}$ is given by $\nu = \dim V = (\dim V_0, \dots, \dim V_n)$.

Given $V \in \mathcal{V}$, let E_V be the space of representations of Q with underlying vector space V . That is,

$$E_V = \bigoplus_{\rho \in Q_1} \text{Hom}(V_{t(\rho)}, V_{h(\rho)})$$

For any subset Q'_1 of Q_1 , let E_{V,Q'_1} be the subspace of E_V consisting of all vectors $x = (x_\rho)$ such that $x_\rho = 0$ whenever $\rho \notin Q'_1$. The algebraic group $G_V = \prod_i \text{Aut}(V_i)$ acts on E_V and E_{V,Q'_1} by

$$(g, x) = ((g_i), (x_\rho)) \mapsto gx$$

$$= (x'_\rho) = (g_{h(\rho)} x_\rho g_{t(\rho)}^{-1})$$

Define the function $\varepsilon: Q_1 \rightarrow \{-1, 1\}$ by $\varepsilon(\rho) = 1$ for all $\rho \in \Omega$ and $\varepsilon(\rho) = -1$ for all $\rho \in \bar{\Omega}$. Let $\langle \cdot, \cdot \rangle$ be the nondegenerate, G_V -invariant, symplectic form on E_V with values in \mathbb{C} defined by

$$\langle x, y \rangle = \sum_{\rho \in Q_1} \varepsilon(\rho) \text{tr}(x_\rho y_{\bar{\rho}})$$

Note that E_V can be considered as the cotangent space of $E_{V,\Omega}$ under this form.

The moment map associated to the G_V -action on the symplectic vector space E_V is the map $\psi: E_V \rightarrow \mathfrak{gl}_V = \prod_i \text{End} V_i$, the Lie algebra of GL_V , with i -component $\psi_i: E_V \rightarrow \text{End} V_i$ given by

$$\psi_i(x) = \sum_{\rho \in Q_1, h(\rho)=i} \varepsilon(\rho) x_\rho x_{\bar{\rho}}$$

Definition 1 An element $x \in E_V$ is said to be nilpotent if there exists an $N \geq 1$ such that for any sequence $\rho_1, \rho_2, \dots, \rho_N$ in H satisfying $t(\rho_1) = h(\rho_2)$, $t(\rho_2) = h(\rho_3), \dots, t(\rho_{N-1}) = h(\rho_N)$, the composition $x_{\rho_1} x_{\rho_2} \dots x_{\rho_N}: V_{t(\rho_N)} \rightarrow V_{h(\rho_1)}$ is zero.

Definition 2 Let Λ_V be the set of all nilpotent elements $x \in E_V$ such that $\psi_i(x) = 0$ for all $i \in I$.

A subset of an algebraic variety is said to be “constructible” if it is obtained from subvarieties from a finite number of the usual set-theoretic operations. A function $f: A \rightarrow \mathbb{Q}$ on an algebraic variety A is said to be a constructible function if $f^{-1}(a)$ is a constructible set for all $a \in \mathbb{Q}$ and is empty for all but finitely many a . Let $M(\Lambda_V)$ denote the \mathbb{Q} -vector space of all constructible functions on Λ_V . Let $\tilde{M}(\Lambda_V)$ denote the \mathbb{Q} -subspace of $M(\Lambda_V)$ consisting of those functions that are constant on any G_V -orbit in Λ_V .

Let $V, V', V'' \in \mathcal{V}$ such that $\dim V = \dim V' + \dim V''$. Now, suppose that S is an I -graded subspace of V . For $x \in \Lambda_V$ we say that S is x -stable if $x(S) \subset S$. Let $\Lambda_{V, V', V''}$ be the variety consisting of all pairs (x, S) where $x \in \Lambda_V$ and S is an I -graded x -stable subspace of V such that $\dim S = \dim V''$. Now, if we fix some isomorphisms $V/S \cong V', S \cong V''$, then x induces elements $x' \in \Lambda_{V'}$ and $x'' \in \Lambda_{V''}$. We then have the maps

$$\Lambda_{V'} \times \Lambda_{V''} \xleftarrow{p_1} \Lambda_{V, V', V''} \xrightarrow{p_2} \Lambda_V$$

where $p_1(x, S) = (x', x'')$, $p_2(x, S) = x$.

For a holomorphic map π between complex varieties A and B , let $\pi_!$ denote the map between the spaces of constructible functions on A and B given by

$$(\pi_! f)(y) = \sum_{a \in \mathbb{Q}} a \chi(\pi^{-1}(y) \cap f^{-1}(a))$$

Let π^* be the pullback map from functions on B to functions on A acting as $\pi^* f(y) = f(\pi(y))$. We then define a map

$$\tilde{M}(\Lambda_{V'}) \times \tilde{M}(\Lambda_{V''}) \rightarrow \tilde{M}(\Lambda_V) \quad [1]$$

by $(f', f'') \mapsto f' * f''$ where

$$f' * f'' = (p_2)_! p_1^*(f' \times f'')$$

Here $f' \times f'' \in \tilde{M}(\Lambda_{V'} \times \Lambda_{V''})$ is defined by $(f' \times f'')(x', x'') = f'(x')f''(x'')$. The map [1] is bilinear and defines an associative \mathbb{Q} -algebra structure on $\oplus_{V'} \tilde{M}(\Lambda_{V'})$ where V' is the object of \mathcal{V} defined by $V'_i = C^{V_i}$.

There is a unique algebra homomorphism $\kappa: \mathcal{U}^+ \rightarrow \oplus_{V'} \tilde{M}(\Lambda_{V'})$ such that $\kappa(e_i)$ is the function on the point Λ_{V^i} with value 1. Then κ restricts to a map $\kappa_\nu: \mathcal{U}_\nu^+ \rightarrow \tilde{M}(\Lambda_{V^\nu})$. It can be shown that $\kappa_{p_i}(e_i^p/p!)$ is the function 1 on the point $\Lambda_{V^{p_i}}$ for $i \in Q_0, p \in \mathbb{Z}_{\geq 0}$.

Let $M_{\mathbb{Z}}(\Lambda_V)$ be the set of all functions in $\tilde{M}(\Lambda_V)$ that take on only integer values. One can show that if

$f' \in \tilde{M}_{\mathbb{Z}}(\Lambda_{V'})$ and $f'' \in \tilde{M}_{\mathbb{Z}}(\Lambda_{V''})$, then $f' * f'' \in \tilde{M}_{\mathbb{Z}}(\Lambda_V)$ in the setup of [1]. Thus $\kappa_\nu(\mathcal{U}_{\mathbb{Z}, \nu}^+) \subseteq \tilde{M}_{\mathbb{Z}}(\Lambda_{V^\nu})$.

Let $\text{Irr} \Lambda_V$ denote the set of irreducible components of Λ_V . The following proposition was conjectured by Lusztig and proved by him in the affine (and finite) case. The general case was proved by Kashiwara and Saito.

Proposition 2 For any $\nu \in (\mathbb{Z}_{\geq 0})^{Q_0}$, we have $\dim \mathcal{U}_\nu^+ = \#\text{Irr} \Lambda_{V^\nu}$.

We then have the following important result due to Lusztig.

Theorem 4 Let $\nu \in (\mathbb{Z}_{\geq 0})^{Q_0}$. Then,

- (i) For any $Z \in \text{Irr} \Lambda_{V^\nu}$, there exists a unique $f_Z \in \kappa_\nu(\mathcal{U}_{\mathbb{Z}, \nu}^+)$ such that f_Z is equal to 1 on an open dense subset of Z and equal to zero on an open dense subset of $Z' \in \text{Irr} \Lambda_{V^\nu}$ for all $Z' \neq Z$.
- (ii) $\{f_Z \mid Z \in \text{Irr} \Lambda_{V^\nu}\}$ is a \mathbb{Q} -basis of $\kappa_\nu(\mathcal{U}_\nu^+)$.
- (iii) $\kappa_\nu: \mathcal{U}_\nu^+ \rightarrow \kappa_\nu(\mathcal{U}_\nu^+)$ is an isomorphism.
- (iv) Define $[Z] \in \mathcal{U}_\nu^+$ by $\kappa_\nu([Z]) = f_Z$. Then $B_\nu = \{[Z] \mid Z \in \text{Irr} \Lambda_{V^\nu}\}$ is a \mathbb{Q} -basis of \mathcal{U}_ν^+ .
- (v) $\kappa_\nu(\mathcal{U}_{\mathbb{Z}, \nu}^+) = \kappa_\nu(\mathcal{U}_\nu^+) \cap \tilde{M}_{\mathbb{Z}}(\Lambda_{V^\nu})$.
- (vi) B_ν is a \mathbb{Z} -basis of $\mathcal{U}_{\mathbb{Z}, \nu}^+$.

From this theorem, we see that $B = \sqcup_\nu B_\nu$ is a \mathbb{Q} -basis of \mathcal{U}^+ , which is called the “semicanonical basis.” This basis has many remarkable properties. One of these properties is as follows. Via the algebra involution of the entire universal enveloping algebra \mathcal{U} of \mathfrak{g} given on the Chevalley generators by $e_i \mapsto f_i, f_i \mapsto e_i$ and $h \mapsto -h$ for h in the Cartan subalgebra of \mathfrak{g} , one obtains from the results of this section a semicanonical basis of \mathcal{U}^- , the lower half of the universal enveloping algebra of \mathfrak{g} . For any irreducible highest-weight integrable representation V of \mathcal{U} (or, equivalently, \mathfrak{g}), let $v \in V$ be a nonzero highest-weight vector. Then the set

$$\{bv \mid b \in B, bv \neq 0\}$$

is a \mathbb{Q} -basis of V , called the semicanonical basis of V . Thus, the semicanonical basis of \mathcal{U}^- is simultaneously compatible with all irreducible highest-weight integrable modules. There is also a way to define the semicanonical basis of a representation directly in a geometric way. This is the subject of the next subsection.

One can also obtain a geometric realization of the upper part \mathcal{U}^+ of the quantum group in a similar manner using perverse sheaves instead of constructible functions. This construction yields the canonical basis of the associated quantum group (a q -deformation of the universal enveloping algebra) which also has many remarkable properties and is closely related to the theory of crystal bases.

Nakajima's Quiver Varieties

We introduce here a description of the quiver varieties first presented by Nakajima. They yield a geometric realization of the irreducible highest-weight representations of simply-laced Kac–Moody algebras. The construction was motivated by the work of Kronheimer and Nakajima on solutions to the anti-self-dual Yang–Mills equations on ALE gravitational instantons (see Instantons: Topological Aspects).

Definition 3 For $\mathbf{v}, \mathbf{w} \in \mathbb{Z}_{\geq 0}^I$, choose I -graded vector spaces V and W of graded dimensions \mathbf{v} and \mathbf{w} , respectively. Then define

$$\Lambda \equiv \Lambda(\mathbf{v}, \mathbf{w}) = \Lambda_V \times \bigoplus_{i \in I} \text{Hom}(V_i, W_i)$$

Definition 4 Let $\Lambda^{\text{st}} = \Lambda(\mathbf{v}, \mathbf{w})^{\text{st}}$ be the set of all $(x, t) \in \Lambda(\mathbf{v}, \mathbf{w})$ satisfying the following condition: if $S = (S_i)$ with $S_i \subset V_i$ is x -stable and $t_i(S_i) = 0$ for $i \in I$, then $S_i = 0$ for $i \in I$.

The group G_V acts on $\Lambda(\mathbf{v}, \mathbf{w})$ via

$$(g, (x, t)) \mapsto ((g_{h(\rho)} x_{\rho} g_{t(\rho)}^{-1}), (t_i g_i^{-1}))$$

and the stabilizer of any point of $\Lambda(\mathbf{v}, \mathbf{w})^{\text{st}}$ in G_V is trivial. We then make the following definition.

Definition 5 Let $\mathcal{L} \equiv \mathcal{L}(\mathbf{v}, \mathbf{w}) = \Lambda(\mathbf{v}, \mathbf{w})^{\text{st}} / G_V$.

We should note that while the above definition and other constructions in this article are algebraic, there are also more geometric ways of looking at quiver varieties. In particular, the space

$$M(\mathbf{v}, \mathbf{w}) = \left(\bigoplus_{\rho \in Q_1} \text{Hom}(V_{t(\rho)}, V_{h(\rho)}) \right) \oplus \left(\bigoplus_{i \in I} \text{Hom}(W_i, V_i) \oplus \text{Hom}(V_i, W_i) \right)$$

has a natural hyper-Kähler metric and one can consider a hyper-Kähler quotient by the group $\prod U(V_i)$. The variety $\mathcal{L}(\mathbf{v}, \mathbf{w})$ is a Lagrangian subvariety of (and is homotopic to) this hyper-Kähler quotient. In the case $\mathfrak{g} = \mathfrak{sl}_n$, the varieties involved are closely related to flag varieties.

Let $\mathbf{w}, \mathbf{v}, \mathbf{v}', \mathbf{v}'' \in \mathbb{Z}_{\geq 0}^I$ be such that $\mathbf{v} = \mathbf{v}' + \mathbf{v}''$. Consider the maps

$$\begin{aligned} \Lambda(\mathbf{v}'', 0) \times \Lambda(\mathbf{v}', \mathbf{w}) &\xrightarrow{p_1} \tilde{F}(\mathbf{v}, \mathbf{w}; \mathbf{v}'') \\ &\xrightarrow{p_2} F(\mathbf{v}, \mathbf{w}; \mathbf{v}'') \xrightarrow{p_3} \Lambda(\mathbf{v}, \mathbf{w}) \end{aligned} \quad [2]$$

where the notation is as follows. A point of $F(\mathbf{v}, \mathbf{w}; \mathbf{v}'')$ is a point $(x, t) \in \Lambda(\mathbf{v}, \mathbf{w})$ together with an I -graded, x -stable subspace S of V such that

$\dim S = \mathbf{v}' = \mathbf{v} - \mathbf{v}''$. A point of $\tilde{F}(\mathbf{v}, \mathbf{w}; \mathbf{v}'')$ is a point (x, t, S) of $F(\mathbf{v}, \mathbf{w}; \mathbf{v}'')$ together with a collection of isomorphisms $R'_i: V'_i \cong S_i$ and $R''_i: V''_i \cong V_i/S_i$ for each $i \in I$. Then we define $p_2(x, t, S, R', R'') = (x, t, S)$, $p_3(x, t, S) = (x, t)$ and $p_1(x, t, S, R', R'') = (x'', x', t')$ where x'', x', t' are determined by

$$\begin{aligned} R'_{h(\rho)} x'_{\rho} &= x_{\rho} R'_{t(\rho)}: V'_{t(\rho)} \rightarrow S_{h(\rho)} \\ t'_i &= t_i R'_i: V'_i \rightarrow W_i \\ R''_{h(\rho)} x''_{\rho} &= x_{\rho} R''_{t(\rho)}: V''_{t(\rho)} \rightarrow V_{h(\rho)}/S_{h(\rho)} \end{aligned}$$

It follows that x' and x'' are nilpotent.

Lemma 1 One has

$$(p_3 \circ p_2)^{-1}(\Lambda(\mathbf{v}, \mathbf{w})^{\text{st}}) \subset p_1^{-1}(\Lambda(\mathbf{v}'', 0) \times \Lambda(\mathbf{v}', \mathbf{w})^{\text{st}})$$

Thus, we can restrict [2] to Λ^{st} , forget the $\Lambda(\mathbf{v}'', 0)$ -factor and consider the quotient by G_V and $G_{V'}$. This yields the diagram

$$\mathcal{L}(\mathbf{v}', \mathbf{w}) \xleftarrow{\pi_1} \mathcal{F}(\mathbf{v}, \mathbf{w}; \mathbf{v} - \mathbf{v}') \xrightarrow{\pi_2} \mathcal{L}(\mathbf{v}, \mathbf{w}) \quad [3]$$

where

$$\begin{aligned} \mathcal{F}(\mathbf{v}, \mathbf{w}, \mathbf{v} - \mathbf{v}') \\ \stackrel{\text{def}}{=} \{(x, t, S) \in F(\mathbf{v}, \mathbf{w}; \mathbf{v} - \mathbf{v}') \mid (x, t) \in \Lambda(\mathbf{v}, \mathbf{w})^{\text{st}}\} / G_V \end{aligned}$$

Let $M(\mathcal{L}(\mathbf{v}, \mathbf{w}))$ be the vector space of all constructible functions on $\mathcal{L}(\mathbf{v}, \mathbf{w})$. Then define maps

$$\begin{aligned} h_i &: M(\mathcal{L}(\mathbf{v}, \mathbf{w})) \rightarrow M(\mathcal{L}(\mathbf{v}, \mathbf{w})) \\ e_i &: M(\mathcal{L}(\mathbf{v}, \mathbf{w})) \rightarrow M(\mathcal{L}(\mathbf{v} - \mathbf{e}^i, \mathbf{w})) \\ f_i &: M(\mathcal{L}(\mathbf{v} - \mathbf{e}^i, \mathbf{w})) \rightarrow M(\mathcal{L}(\mathbf{v}, \mathbf{w})) \end{aligned}$$

by

$$\begin{aligned} h_i f &= u_i f \\ e_i f &= (\pi_1)_!(\pi_2^* f) \\ f_i g &= (\pi_2)_!(\pi_1^* g) \end{aligned}$$

Here

$$u = {}^t(u_0, \dots, u_n) = w - C\mathbf{v}$$

where C is the Cartan matrix of \mathfrak{g} and we are using diagram 3 with $\mathbf{v}' = \mathbf{v} - \mathbf{e}^i$ where \mathbf{e}^i is the vector whose components are given by $e_j^i = \delta_{ij}$.

Now let φ be the constant function on $\mathcal{L}(0, \mathbf{w})$ with value 1. Let $L(\mathbf{w})$ be the vector space of functions generated by acting on φ with all possible combinations of the operators f_i . Then let $L(\mathbf{v}, \mathbf{w}) = M(\mathcal{L}(\mathbf{v}, \mathbf{w})) \cap L(\mathbf{w})$.

Proposition 3 The operators e_i, f_i, h_i on $L(\mathbf{w})$ provide it with the structure of the irreducible highest-weight

integrable representation of \mathfrak{g} with highest weight $\sum_{i \in Q_0} w_i \omega_i$. Each summand of the decomposition $L(w) = \bigoplus_v L(v, w)$ is a weight space with weight $\sum_{i \in Q_0} w_i \omega_i - v_i \alpha_i$. Here the ω_i and α_i are the fundamental weights and simple roots of \mathfrak{g} , respectively.

Let $Z \in \text{Irr} \mathcal{L}(v, w)$ and define a linear map $T_Z: L(v, w) \rightarrow \mathbb{C}$ that associates to a constructible function $f \in L(v, w)$ the (constant) value of f on a suitable open dense subset of Z . The fact that $L(v, w)$ is finite dimensional allows us to take such an open set on which any $f \in L(v, w)$ is constant. So we have a linear map

$$\Phi: L(v, w) \rightarrow \mathbb{C}^{\text{Irr} \mathcal{L}(v, w)}$$

Then we have the following proposition.

Proposition 4 *The map Φ is an isomorphism; for any $Z \in \text{Irr} \mathcal{L}(v, w)$, there is a unique function $g_Z \in L(v, w)$ such that for some open dense subset O of Z we have $g_Z|_O = 1$ and for some closed G_V -invariant subset $K \subset \mathcal{L}(v, w)$ of dimension $< \dim \mathcal{L}(v, w)$ we have $g_Z = 0$ outside $Z \cup K$. The functions g_Z for $Z \in \text{Irr} \mathcal{L}(v, w)$ form a basis of $L(v, w)$.*

Additional Topics

To conclude, we have given here a brief overview of some topics related to finite-dimensional algebras and quivers. There is much more to be found in the literature. For basics on associative algebras and their representations, the reader may consult introductory texts on abstract algebra such as Lang (2002). For further results (and their proofs) on Ringel–Hall algebras see the papers of Ringel (1990a, b, 1993, 1995, 1996) and of Green (1995) and the references cited therein. The reader interested in species, which extend many of these results to non-simply-laced Lie algebras, should consult Dlab and Ringel (1976).

The book by Lusztig (1993) covers the quiver varieties of Lusztig and canonical bases. Canonical bases are closely related to crystal bases and crystal graphs (see Hong and Kang (2002) for an overview of these topics). In fact, the set of irreducible components of the quiver varieties of Lusztig and Nakajima can be endowed with the structure of a crystal graph in a purely geometric way (see Kashiwara and Saito (1997) and Saito (2002)). Many results on Nakajima's quiver varieties can be found in the original papers (Nakajima 1994, 1998). The overview article (Nakajima 1996) is also useful.

Quiver varieties can also be used to give geometric realizations of tensor products of representations (see Malkin (2002, 2003), Nakajima (2001), and Savage (2003)) and finite-dimensional representations of quantum affine Lie algebras (see Nakajima (2001)). This is just a select few of the many applications of quiver varieties. Much more can be found in the literature.

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See also: Instantons: Topological Aspects.

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Finite Group Symmetry Breaking

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Introduction

It is a commonplace situation that symmetric laws of Nature give rise to physical states which are not symmetric. States related by symmetry operations are equivalent, but still nature selects one of them.

As an example, consider a ferromagnetic system of interacting spins with no external magnetic field. The “up” and “down” states are equivalent, but one of the two is chosen: the interaction makes states with agreeing spin orientation (and therefore macroscopic magnetization) energetically preferred, and fluctuations will decide which state is actually chosen by a given sample.

Finite group symmetry is also commonplace in physics, in particular through crystallographic groups occurring in condensed matter physics – but also through the inversions (C , P , T and their combinations) occurring in high-energy physics and field theory.

The breaking of finite group symmetry has thus been thoroughly studied, and general approaches exist to investigate it in mathematically precise terms with physical counterparts. In particular, a widely applicable approach is provided by the Landau theory of phase transitions – whose mathematical counterpart resides in the realm of equivariant singularity and bifurcation theory. In Landau theory, the state of a system is described by a finite-dimensional variable (the “order parameter”), and physical states correspond to minima of a potential, invariant under a group.

In this article we describe the basics of symmetry breaking analysis for systems described by a symmetric polynomial; in particular, we

discuss generic symmetry breakings, that is, those determined by the symmetry properties themselves and independent of the details of the polynomial describing a concrete system. We also discuss how the plethora of invariant polynomials can be to some extent reduced by means of changes of coordinates, that is, how one can reduce to consider certain types of polynomials with no loss of generality. Finally, we will give some indications on extension of this theory, that is, on how one deals with symmetry breakings for more general groups and/or more general physical systems.

Basic Notions

Finite Groups

A finite group (G, \circ) is a finite set G of elements $\{g_0, \dots, g_N\}$ equipped with a composition law \circ , and such that the following conditions hold:

1. for all $g, h \in G$ the composition $g \circ h$ belongs to G , that is, $g \circ h \in G$;
2. the composition is associative, that is, $(g \circ h) \circ k = g \circ (h \circ k)$ for all $g, h, k \in G$;
3. there is an element in G – which we will denote as e – which is the identity for the action of \circ on G , that is, $e \circ g = g = g \circ e$ for all $g \in G$; and
4. for each $g \in G$ there is an element g^{-1} which is the inverse of g , that is, $g^{-1} \circ g = e = g \circ g^{-1}$.

In the following, we omit the symbol \circ , that is, we write gh to mean $g \circ h$. Similarly, we usually write simply G for the group, rather than (G, \circ) .

Given a subset $H \subseteq G$, this is a subgroup of (G, \circ) if (H, \circ) satisfies the group axioms (1)–(4) above. Note that this implies that $e \in H$ whenever H is a subgroup, and $\{e\}$ is a subgroup. Subgroups not coinciding with the whole G and with $\{e\}$ are said to be “proper.”

Given two elements g, h we say that ghg^{-1} is the conjugate of h by g . The conjugate of a subgroup $H \subseteq G$ by $g \in G$ is the subgroup of elements conjugated to elements of H , $gHg^{-1} = \{(ghg^{-1}), h \in H\}$.

Group Action

In physics, one is usually interested in a realization of an abstract group as a group of transformations in some set X ; in physical applications, this is usually a (possibly, function) space or a manifold, and we refer to elements of X as “points.” That is, there is a map $\rho: G \rightarrow \text{End}(X)$ from G to the group of endomorphisms of X , such to preserve the composition law:

$$\rho(g) \cdot \rho(h) = \rho(g \circ h) \quad \forall g, h \in G$$

In this case, we say that we have a “representation” of the abstract group G acting in the “carrier” space or manifold X ; we also say that X is a G -space or G -manifold. We often denote by the same letter the abstract element and its representation, that is, write simply g for $\rho(g)$ and G for $\rho(G)$. (In many physically relevant cases, but not necessarily, X has a linear structure and we consider linear endomorphisms. In this case, we sometimes write T_g for the linear operator representing g .)

If $x \in X$ is a point in X , the G -orbit $G(x)$ is the set of points to which x is mapped under G , that is,

$$G(x) = \{y \in X: y = gx, g \in G\} \subseteq X$$

Belonging to the same orbit is obviously an equivalence relation, and partitions X into equivalence classes. The “orbit space” for the G action on X , also denoted as $\Omega = X/G$, is the set of these equivalence classes. It corresponds, in physical terms, to considering X modulo identification of elements related by the group action.

For any point $x \in X$, the “isotropy (sub)group” G_x is the set of elements leaving x fixed,

$$G_x = \{g \in G: gx = x\} \subseteq G$$

Points on the same G -orbit have conjugated isotropy subgroups: indeed, $y = gx$ implies immediately that $G_y = gG_xg^{-1}$.

When a topology is defined on X , the problem arises if the G -action preserves it; if this is the case, we say that the G -action is “regular.” In the case of a compact Lie group (and *a fortiori* for a finite group) we are guaranteed the action is regular. (A physically relevant example of nonregular action is provided by the irrational flow on a torus. In this case $G = \mathbb{R}$, realized as the time t irrational flow on the torus $X = T^k$.)

Spontaneous Symmetry Breaking

Let us now consider the case of physical systems whose state is described by a point x in the G -space or G -manifold X , with G a group acting by smooth mappings $g: X \rightarrow X$. In physical problems, G quite often acts by linear and orthogonal transformations. (If this is not the case, the Palais–Mostow theorem guarantees that, for suitable groups (including in particular the finite ones) we can reduce to this case upon embedding X into a suitably larger carrier space Y .)

Usually, G represents physical equivalence of states, and G -orbits are collections of physically equivalent states. A point which is G -invariant, that is, such that $G_x = G$, is called “symmetric” for short.

Let Φ be a scalar function (potential) defined on X , $\Phi: X \rightarrow \mathbb{R}$, possibly depending on some parameter μ , such that the physical state corresponds to critical points – usually the (local) minima – of Φ .

A concrete example is provided by the case where Φ is the Gibbs free energy; more generally, this is the framework met in the Landau theory of phase transitions (Landau 1937, Landau and Lifshitz 1958).

We are interested in the case where Φ is invariant under the group action, or briefly G -invariant, that is, where

$$\Phi(gx) = \Phi(x) \quad \forall x \in X, \forall g \in G \quad [1]$$

A critical point x such that $G_x = G$ is a symmetrical critical point. If G_x is strictly smaller than G , then x is a symmetry-breaking critical point.

If a physical system corresponds to a nonsymmetrical critical point, we have a spontaneous symmetry breaking: albeit the physical laws (the potential function Φ) are symmetric, the physical state (the critical point for Φ) breaks the symmetry and chooses one of the G -equivalent critical points.

It follows from [1] that the gradient of Φ is covariant under G . If $y = gx$, then the differential (Dg) of the map $g: X \rightarrow X$ is a linear map between the corresponding tangent spaces, $(Dg): T_x X \rightarrow T_y X$. The covariance amounts, with η the Riemannian metric in X , to $(\eta^{ij} \partial_j \Phi)(gx) = [(Dg)_k^i \eta^{km} \partial_m \Phi](x)$; this is also written compactly, with obvious notation, as

$$(\nabla \Phi)(gx) = (Dg)[(\nabla \Phi)(x)] \quad [2]$$

(in the case of euclidean spaces ($\eta = \delta$) and linear actions described by matrices T_g , the covariance condition reduces to $(\nabla \Phi)^i(T_g x) = (T_g)_j^i [(\nabla \Phi)^j(x)]$). As (Dg) is a linear map, $(\nabla \Phi)(x) = 0$ implies the vanishing of $\nabla \Phi$ at all points on the G -orbit of x .

We conclude that critical points of a G -invariant potential come in G -orbits: if x is a critical point for

Φ , then each $y \in G(x)$ is also a critical point for Φ . We speak therefore of critical orbits for Φ .

It is thus possible (thanks to the regularity of the G -action), and actually convenient, to study spontaneous symmetry breaking in the orbit space $\Omega = X/G$ rather than in the carrier manifold X (Michel 1971).

If G describes physical equivalence, physical states whose symmetries are G -conjugated should be seen as physically equivalent. An equivalence class of isotropy types under conjugation will be said to be a symmetry type. We are thus interested, given a G -invariant polynomial Φ , to know the symmetry types of its critical points. We denote symmetry types as $[H] = \{gHg^{-1}\}$, and say that $[H] < [K]$ if a group conjugated to H is strictly contained in a group conjugated to K .

As we have seen, points on the same G -orbit have the same symmetry type. On the other hand, points on different G -orbits can have the same isotropy type (e.g., for the standard action of $O(n)$ in \mathbb{R}^n , all collinear nonzero points will have the same isotropy subgroup but will lie on distinct group orbits).

G-Invariant Polynomials

Consider a finite group G acting in X . (Many of the notions and results mentioned in this section have a much wider range of applicability.) We look at the ring of G -invariant scalar polynomials in x^1, \dots, x^n .

By the Hilbert basis theorem, there is a set $\{J_1(x), \dots, J_k(x)\}$ of G -invariant homogeneous polynomials of degrees $\{d_1, \dots, d_k\}$ such that any G -invariant polynomial $\Phi(x)$ can be written as a polynomial in the $\{J_1, \dots, J_k\}$, that is,

$$\Phi(x) = \Psi[J_1(x), \dots, J_k(x)] \quad [3]$$

with Ψ a polynomial. (A similar theorem holds for smooth functions.)

The algebra of G -invariant polynomials is finitely generated, that is, we can choose k finite. When the J_a are chosen so that none of them can be written as a polynomial of the others and r has the smallest possible value (this value depends on G), we say that they are a minimal integrity basis (MIB). (Note that some of the J_a could be written as nonpolynomial functions of the others, and the J_α could satisfy polynomial relations. For example, consider the group Z_2 acting in \mathbb{R}^2 via $g: (x, y) \rightarrow (-x, -y)$; an MIB is made of $J_1(x, y) = x^2$, $J_2(x, y) = y^2$, and $J_3(x, y) = xy$. None of these can be written as a polynomial function of the others, but $J_1 J_2 = J_3^2$.) In this case, we say that the $\{J_a\}$ are a set of basic invariants for G . There is obviously some arbitrariness in the choice of the J_a in an MIB, but the

degrees $\{d_1, \dots, d_k\}$ of $\{J_1, \dots, J_k\}$ are fixed by G . (In mathematical terms, they are determined through the Poincaré series of the graded algebra P_G of G -invariant polynomials.)

We will henceforth assume that we have chosen an MIB, with elements $\{J_1, \dots, J_k\}$ of degrees $\{d_1, \dots, d_k\}$ in x , say with $d_1 \leq d_2 \leq \dots \leq d_k$.

When the elements of an MIB for G are algebraically independent, we say that the MIB is regular; if G admits a regular MIB we say that G is coregular.

An algebraic relation between elements J_α of the MIB is said to be a relation of the first kind. The algebraic relations among the J are a set of polynomials in $\{J_1, \dots, J_r\}$, which are identically zero when seen as polynomials in x . If there are algebraic relations among these, they are called relations of the second kind, and so on. A theorem by Hilbert guarantees that the chain of relations has finite maximal length. (This is the homological dimension of the graded algebra P_G mentioned above.)

In the following, we will consider a matrix built with the gradients of basic invariants, the \mathcal{P} -matrix (Sartori). This is defined as

$$\mathcal{P}_{ib}(x) := \langle \nabla J_i(x), \nabla J_b(x) \rangle \quad [4]$$

with $\langle \cdot, \cdot \rangle$ the scalar product in $T_x X$.

The gradient of an invariant is necessarily a covariant quantity; the scalar product of two covariant quantities is an invariant one, and thus can be expressed again in terms of the basic invariants. Thus, the \mathcal{P} -matrix can always be written in terms of the basic invariants themselves.

Geometry of Group Action

The use of an MIB allows to introduce a map $J: x \rightarrow \{J_1(x), \dots, J_k(x)\}$ from X to a subset P of \mathbb{R}^k . If the MIB is regular, $P = \mathbb{R}^k$, while if the J_i satisfy some relation then $P \subset \mathbb{R}^k$ is the submanifold satisfying the corresponding relations. The manifold P is isomorphic to the orbit space $\Omega = X/G$ (the isomorphism being realized by the J map) and provides a more convenient framework to study Ω .

As mentioned above, on physical terms we are mainly interested in the orbit space up to equivalence of symmetry type. The set of points in X (of orbits in Ω) with the same symmetry type will be called a G -stratum in X (a G -stratum in Ω); the G -stratum of the point x will be denoted as $\sigma(x) \subset X$ (the G -stratum of the orbit ω as $\Sigma(\omega) \subset \Omega$). (The notion of stratum was introduced by Whitney in topology; a stratified manifold is a set which can be decomposed as the disjoint union of smooth

manifolds of different dimensions, the topological (or Whitney) strata: $M = \bigcup M^k$, with $M^k \subset \partial M^j$ for all $k < j$.)

It results that the G -stratification is compatible with the topological stratification. Indeed, P is a semialgebraic (i.e., it is defined by algebraic equalities and inequalities) stratified manifold in \mathbb{R}^k ; the image of any G -stratum in Ω belongs to a single topological stratum in P , and topological strata in P are the union of images of G -strata in Ω .

Moreover, the subgroup relations correspond to bordering relations between G -strata: if $[G_x] < [G_y]$, then $\sigma(y) \in \partial\sigma(x)$ and (with ω_x the orbit of x) $\Sigma(\omega_y) \in \partial\Sigma(\omega_x)$.

There is a stratum, called the principal stratum σ_0 , which corresponds to minimal isotropy, open and dense in X ; similarly, the principal stratum Σ_0 is open and dense in Ω .

Landau Polynomial

In the Landau (1937) theory of phase transitions, the state of the system under study is described by a G -invariant polynomial $\Phi: X \rightarrow \mathbb{R}$ having a critical point in the origin, with at least some of its coefficients – in particular those controlling the stability of the zero critical point – depending on external control parameters (usually, $X = \mathbb{R}^n$ and $G \subseteq O(n)$; in particular, in solid-state physics G is a crystallographic group). This should be chosen as the most general G -invariant polynomial of the lowest degree ℓ sufficient to ensure thermodynamic stability; in mathematical terms, this amounts to the requirement that there is some open set \mathcal{B} containing the origin and such that – for all values of the control parameters – $\nabla\Phi$ points inwards at all points of $\partial\mathcal{B}$ (i.e., \mathcal{B} is invariant under the gradient flow of Φ). If the polynomials in the MIB are of degree $d_1 \leq d_2 \leq \dots \leq d_r$, then usually $\ell = 2d_r$.

The G -invariance of Φ and the results recalled above mean that we can always write it in terms of the polynomials in an MIB for G as in [3], $\Phi(x) = \Psi[J(x)]$.

The discussion of previous sections shows that we can study symmetry breakings for $\Phi: X \rightarrow \mathbb{R}$ by studying critical points of $\Psi: P \rightarrow \mathbb{R}$; in other words, Landau theory can be worked out in the G -orbit space $\Omega := M/G$. The polynomial Ψ – providing a representation of the Landau polynomial in the orbit space – will also be called Landau–Michel polynomial. (Louis Michel (1923–1999) pioneered the use of orbit space techniques in physics and nonlinear dynamics, originally motivated by the study of hadronic interactions.)

In this way, the evaluation of the map $\Phi: X \rightarrow \mathbb{R}$ is, in principle, substituted by evaluation of two maps, $J: X \rightarrow P$ and $\Psi: P \rightarrow \mathbb{R}$. However, if, as in Landau theory, we have to consider the most general G -invariant polynomial on X , we can just consider the most general polynomial on P .

Critical Points of the Landau Polynomial and Geometry of Orbit Space

The G -invariance has consequences on the critical points of Φ . We have already seen one such consequence: critical points come in G -orbits.

However, this is not all. Indeed, G -invariance enforces the presence of a certain set $\chi(G) \in X$ of critical points, and conversely if we look for points which are critical under any G -invariant potential, these are precisely the points in $\chi(G)$; the critical points on $\chi(G)$ correspond to critical orbits which we call principal critical orbits.

The set $\chi(G)$ can be determined on the basis of the geometry of the G -action. (A trivial example is provided by $X = \mathbb{R}$ and $G = \mathbb{Z}_2$ acting via $g: x \rightarrow -x$; any even function has a critical point in zero, and albeit even functions can, and in general will, have nonzero critical points, this is the only critical point common to all the even functions.) Indeed (Michel 1971): *an orbit ω is a principal critical orbit if and only if it is isolated in its stratum.*

For the linear orthogonal group actions in \mathbb{R}^n often occurring in physics, no nonzero point or orbit can be isolated in its stratum. However, we can quotient out the radial degeneracy and work on $X = S^{n-1} \subset \mathbb{R}^n$. In this case, a G -orbit ω_1 in S^{n-1} which is isolated in its stratum corresponds to a one-dimensional family $\{\omega_r\}$ of G -orbits in \mathbb{R}^n (call X_0 the corresponding submanifold in X); the gradient of Φ at $x \in X_0$ points along $T_x X_0$. We can thus reduce to consider the restriction Φ_0 of the potential Φ to X_0 . (See also the reduction lemma of Golubitsky and Stewart in this context.)

Correspondingly, if $P_0 \subset P$ is the submanifold in P image of X_0 , that is, $P_0 = J(X_0)$, we can reduce to consider the restriction Ψ_0 of Ψ to P_0 .

As these become one-dimensional problems, general results are available. In particular, one can provide general conditions ensuring the existence of one-dimensional branches of symmetry-breaking solutions bifurcating from zero along any such X_0 or P_0 ; this is also known as the equivariant branching lemma of Cicogna and Vanderbauwhede.

Reduction of the Landau Potential

In realistic problems, Φ quickly becomes extremely complicated, that is, it includes a high number of terms and therefore of coefficients. A thorough study of different symmetry-breaking patterns, that is, of the symmetry type of minima of Φ for different values of these coefficients and of the external control parameter, is in this case a prohibitive task. It is possible to reduce the generality of the Landau polynomial with no loss of generality for the corresponding physical problem. Indeed, a change of coordinates in the X space will produce a formally different – but obviously equivalent – Landau polynomial; it is convenient to use coordinates in which the Landau polynomial is simpler.

A systematic and algorithmic reduction procedure – based on perturbative expansion near the origin – is well known in dynamical systems theory (Poincaré–Birkhoff normal forms), and can be adapted to the reduction of Landau polynomials. (An alternative and more general – but also much more demanding – approach is provided by the spectral sequence approach, also originating in normal-form theory.)

We work near the origin, so that we can assume $X = \mathbb{R}^n$ (with metric η), and for simplicity we also take the case where G acts via a linear representation T_g . We consider changes of coordinates of the (Poincaré) form

$$x^i = y^i + h^i(y) \quad [5]$$

generated by a G -invariant function $H: h^i(y) = \eta^{ij} (\partial H(y) / \partial y^j)$; this guarantees that [5] preserves the G -invariance of Φ . The action of [5] on Φ can be read from its action on the basic invariants J_a . It results

$$\begin{aligned} J_a(x) &= J_a(y) + (\delta J_a)(y) \\ \delta J_a &:= \mathcal{P}_{ab} (\partial H / \partial J_b) \end{aligned} \quad [6]$$

Let us now consider the reduction of an invariant polynomial $\Phi(x) = \Psi(J)$. We write $D_\alpha := \partial / \partial J_\alpha$, and understand that summation over repeated indices is implied. In general,

$$\begin{aligned} \Psi(J) &\rightarrow \Psi(J + \delta J) \\ &= \Psi(J) + \sum_{\alpha=1}^r \frac{\partial \Psi(J)}{\partial J_\alpha} \delta J_\alpha + \dots \end{aligned}$$

where the ellipsis means higher-order terms.

Disregarding higher-order terms and using [6] and [4], we get

$$\delta \Psi = \frac{\partial \Psi}{\partial J_\alpha} \mathcal{P}_{\alpha\beta} \frac{\partial H}{\partial J_\beta} \equiv (D_\alpha \Psi) \mathcal{P}_{\alpha\beta} (D_\beta H) \quad [7]$$

We expand Φ as a sum of homogeneous polynomials, and write $\Phi(x) = \sum_{k=0}^\ell \Phi_k(x)$, where

$\Phi_k(ax) = a^{k+1} \Phi_k(x)$. Also, write $\Psi = \sum_k \Psi_k$, where $\Phi_k(x) := \Psi_k[J(x)]$.

It results that under a change of coordinates [5] generated by $H = H_m$ homogeneous of degree $m+1$, the terms Ψ_k with $k \leq m$ are not changed, while the terms Ψ_{m+p} change according to

$$\begin{aligned} \Psi_{m+p} &\rightarrow \Psi_{m+p} \\ &= \Psi_{m+p} + (D_\alpha \Psi_p) \mathcal{P}_{\alpha\beta} (D_\beta H_m) + \dots \end{aligned} \quad [8]$$

We can then operate sequentially with H_m of degree 3, 4, ...; at each stage (generator H_m), we are not affecting the terms Ψ_k with $k \leq m$. Moreover, we can just consider [8], as higher-order terms are generic and will be taken care of in subsequent steps. (This procedure requires to determine suitable generating functions H_m ; these are obtained as solutions to homological equations.)

In the above, we disregarded the dependence on the control parameters, such as temperature, pressure, magnetic field, etc; that is, we implicitly considered fixed values for these. However, they have to change for a phase transition to take place. If we consider a full range of values – including in particular the critical ones – for the control parameters, say $\lambda \in \Lambda$, we should take care that the concerned quantities and operators are nonsingular uniformly in Λ .

This leads to reduction criteria for the Landau and Landau–Michel polynomials (Gufan). Define, for $i = 1, \dots, k$ the quantities $U_i(J_1, \dots, J_k) := (\partial F / \partial J_s) \mathcal{P}_{si}$.

Reduction Criterion

For $\Phi(x) = \Psi(J_1, \dots, J_k): \mathbb{R}^n \rightarrow \mathbb{R}$ a G -invariant potential depending on physical parameters $\lambda \in \Lambda$, there is a sequence of Poincaré changes of coordinates such that Φ is expressed in the new coordinates y as $\hat{\Phi}(y) = \hat{\Psi}(J)$, where terms which can be written (up to higher-order terms) uniformly in Λ as $\sum_{\alpha=1}^k Q_\alpha(J_1, \dots, J_k) U_\alpha(J_1, \dots, J_k)$, with Q_α polynomials in J_1, \dots, J_k satisfying the compatibility condition $(\partial Q_\beta / \partial J_\alpha) = (\partial Q_\alpha / \partial J_\beta)$, are not present in $\hat{\Psi}$.

Nonstationary and Nonvariational Problems

So far we have considered stationary physical states. In some cases, one is not satisfied with such a description, and wants to study time evolution. A model framework for this is provided by the Ginzburg–Landau equation

$$\dot{x} = f(x) \quad [9]$$

where $f = \eta(\nabla \Phi): X \rightarrow TX$ (see above for notation). In this case, G -invariance of Φ implies equivariance

of [9]. More generally, we can consider [9] for an equivariant smooth f (not necessarily a gradient), that is, $f^i(gx) = (Dg)_j^i f^j(x)$.

In this case, one shows that

$$f(x) \in T_x \sigma(x) \quad [10]$$

so that closures of G -strata are dynamically invariant, and the dynamics can be reduced to them. This is of special interest for the “most singular” strata, that is, those of lower dimension. The reduction lemma and the equivariant branching lemma mentioned above also hold (and were originally formulated) in this context.

The relation [10] also implies that one can project the dynamics [9] in X to a smooth dynamics $\dot{p} = F(p)$ in the orbit space; this satisfies $F[J(x)] = (DJ)[f(x)]$. In the gradient case, this (together with initial conditions) embodies the full dynamics in X , while in the generic case one loses all information about motions along group orbits (note that these correspond to phonon modes).

An orbit ω isolated in its stratum is still an orbit of fixed points for any G -equivariant dynamics in X in the gradient case, while in the generic case it corresponds to a fixed point for F and to relative equilibria (dynamical orbits which belong to a single group orbit) in X . In this case, time averages of physical quantities can be G -invariant for nontrivial relative equilibria.

Extensions and Physical Applications

We have discussed finite group symmetry breaking and focused on polynomial potentials (which can be thought of as Taylor expansions around critical points). For nonfinite groups, and in particular noncompact ones, the situation can be considerably more complicated.

1. An extension of the theory sketched here is provided by Palais' theory, and in particular by his “symmetric criticality principle,” which applies in Hilbert or Banach spaces of sections of a fiber bundle satisfying certain conditions. This is especially relevant in connection with field theory and gauge groups.
2. We focused on the situation discussed in classical physics. Finite group symmetry breaking is of course also relevant in quantum mechanics; this is discussed, for example, in the classical books by Weyl (1931) and Wigner (1959), and in the review by Michel *et al.* (2004).
3. One speaks of “explicit symmetry breaking” when a nonsymmetric perturbation is introduced in a symmetric problem. In the Hamiltonian

case (or in the Lagrangian one for Noether symmetries), Hamiltonian symmetries correspond to conserved quantities, and nonsymmetric perturbations make these become approximate constants of motion.

4. The symmetry of differential equations – as well as symmetric and symmetry-breaking solutions for symmetric equations – can be studied in general mathematical terms (see, e.g., Olver (1986)).
5. Physical applications of the theory discussed here abound in the literature, in particular through the Landau theory of phase transitions. A number of these, together with a deeper discussion of the underlying theory, is given in the monumental review paper by Michel *et al.* (2004).

See also: Central Manifolds, Normal Forms; Compact Groups and Their Representations; Electroweak Theory; Finite Group Symmetry Breaking; Phase Transitions in Continuous Systems; Quasiperiodic Systems; Symmetry and Symmetry Breaking in Dynamical Systems; Symmetry Breaking in Field Theory.

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Finite Weyl Systems

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Introduction

Finite Weyl systems have their applications in various branches of quantum information theory. They are helpful to tame the growth of complexity for a large class of quantum systems: a key discrepancy between classical and quantum systems is the difference in the growth of complexity as one goes to larger and larger systems. This is encountered by simulating a quantum spin system on a computer, for example, with the aim to determine the ground state of a solid-state model of magnetism. For a model of N classical spins, this involves checking the energy for 2^N different configurations, but for a model with quantum spins it requires the solution of an eigenvalue equation in a Hilbert space of dimension 2^N , which is a vastly more difficult problem for large N . For a three-dimensional lattice, three sites each way ($N=27$), this is a problem in 10^8 dimensions, and lattice size 4 leads to utterly untractable 10^{19} dimensions.

It is therefore highly desirable to find ways of treating at least some aspects of large, complex quantum systems without actually having to write out state vectors component by component. States which are invariant under a suitable discrete abelian symmetry group satisfy this condition. They can be characterized by simple combinatorial data, which do not grow exponentially with the system size N . At the same time, the class of these so-called stabilizer states is sufficiently complex to capture some of the key features needed for computation, especially the quantum correlation (entanglement) between subsystems. They have also been shown to be sufficient to generate large quantum error correcting codes.

A further motivation for finite Weyl systems is directly based on constructing quantum error correcting codes from classical coding procedures (see Quantum Error Correction and Fault Tolerance). The “quantization” technique which is used there naturally leads to the structure of finite Weyl systems.

Finite Weyl systems precisely represent quantum versions of discrete abelian symmetry groups. It is a standard procedure to build the quantum version of a symmetry group by an appropriate central extension, or equivalently, to study all its projective

representations: the composition of two symmetry transformations is only preserved up to a phase on the representation Hilbert space. The unitary operators which represent the symmetry transformations are called Weyl operators.

The simplest and most prominent example for a finite Weyl system is given by the three Pauli matrices and the identity. These four unitary operators build a projective representation of the symmetry group of binary vectors $(0,0)$, $(0,1)$, $(1,0)$, $(1,1)$, where the group law is the addition modulo two. The null-vector $(0,0)$ corresponds to the identity, the vector $(0,1)$ is assigned to X , $(1,0)$ corresponds to Z , and $(1,1)$ is mapped to iY . It is not difficult to verify that the product of two Pauli operators preserves the addition of binary vectors up to a phase.

Discrete Weyl systems are deeply related to symplectic geometry for vector spaces over finite fields. The additive structure of the vector space is the underlying abelian symmetry group. The exchange of two Weyl operators within a product produces a phase that is the exponential of an antisymmetric bilinear form, as it is explained in the next section. For irreducible Weyl systems, this antisymmetric form must be symplectic because the Weyl operators generate a full matrix algebra. In particular, this requires that the dimension of the underlying vector space is even. The Pauli matrices are also an example for this more special structure: the binary vectors $(p,q)_{p,q=0,1}$ are a two-dimensional vector space over the field with two elements $\{0,1\}$. The commutation relations for Pauli operators imply that the symplectic form can be evaluated for two binary vectors $(p,q), (p',q')$ according to $pq' - qp' \bmod 2$. It is apparent to interpret the binary vectors (p,q) as points in a discrete phase space, where the first entry corresponds to the momentum and the second to the position. In view of this, discrete Weyl systems serve as a finite-dimensional analog of the canonical commutation relations.

For the generic situation in quantum information theory, an irreducible Weyl system is represented on the Hilbert space describing a system of several single particles. Stabilizer states are left unchanged under the action of a so-called isotropic subgroup which consists of mutually commuting Weyl operators: this kind of invariance is precisely the type of constraint that reduces the complexity for the parametrization of the state. For an efficient description of such states, there are combinatorial techniques available e.g., graph theory.

Operations that preserve the class of stabilizer states (for a particular symmetry group) must be covariant with respect to this symmetry. These operations are called Clifford channels which have far-reaching applications in the theory of quantum error correction. They also allow to take classical coding procedures and turn them into quantum codes: on the classical level, the encoding operation acts on classical phase space as a linear map (additive code). Up to a choice of phases, this induces a quantum channel that preserves the structure of Weyl systems. These codes are called stabilizer codes and have been investigated by many authors (Calderbank *et al.* 1997, Cleve and Gottesman 1996, 1997) (see Quantum Error Correction and Fault Tolerance). In particular, the first quantum error correcting codes belong to this class.

This article is organized as follows. In the next section, the basic mathematical notions are provided, like projective representations, Weyl systems, and irreducibility. Moreover, statements on the main structure of Weyl systems are presented. Next, the notion of Weyl covariant channels (Clifford channels) is introduced and their basic properties are stated. In particular, stronger results for the reversible case are given. The relation between symplectic geometry and reversible Clifford operations on finite Weyl systems is explained. Results on the general structure of stabilizer states and stabilizer codes are given in the penultimate section. Finally, the representation of stabilizer codes in terms of graphs is described.

Finite Weyl Systems

A projective representation of a group Ξ assigns to each group element ξ a unitary operator $w(\xi)$ on a Hilbert space \mathcal{H} such that the group law is preserved up to a phase, that is, the relation

$$w(\xi_1 + \xi_2) = f(\xi_1, \xi_2)w(\xi_1)w(\xi_2) \quad [1]$$

is fulfilled for a phase-valued function f on Ξ^2 . In the following, we denote a projective representation by a triple (w, f, \mathcal{H}) . A finite Weyl system is a projective representation of a finite abelian group. The operators $w(\xi)$ are called Weyl operators and the function f is called the factor system. We refer to the work by Zmud (1971, 1972) for an analysis of projective representations for general abelian groups.

The Weyl algebra $\mathcal{A}(w, f, \mathcal{H})$ associated with a Weyl system (w, f, \mathcal{H}) is the smallest norm-closed subalgebra in the space of bounded operators $\mathcal{B}(\mathcal{H})$ which contains all Weyl operators. If the Weyl algebra coincides with the algebra of all bounded operators, then the Weyl system is called irreducible.

This is equivalent to the fact that each operator that commutes with all Weyl operators must be a multiple of the identity.

In order to analyze the properties of factor systems systematically, we introduce here a few pieces of the cohomology theory of groups. For each positive integer $k=1, 2, 3, \dots$ we introduce the abelian group $C^k(\Xi)$ of k -cochains which consists of all phase-valued functions on Ξ^k . The product and the inverse of k -cochains is defined pointwise. Factor systems are special 2-cochains. Namely, if we consider a Weyl system (w, f, \mathcal{H}) , then associativity implies that the so-called 2-cocycle condition,

$$f(\xi_1 + \xi_2, \xi_3)f(\xi_2, \xi_3)^{-1}f(\xi_1, \xi_2 + \xi_3)^{-1}f(\xi_1, \xi_2) = 1 \quad [2]$$

holds. This property can also be expressed by a coboundary map ∂ which is a group homomorphism from k -cochains to $(k+1)$ -cochains. We consider here the action of the coboundary map on a 1-cochain φ and a 2-cochain f :

$$(\partial\varphi)(\xi_1, \xi_2) := \varphi(\xi_1 + \xi_2)\varphi(\xi_1)^{-1}\varphi(\xi_2)^{-1} \quad [3]$$

$$(\partial f)(\xi_1, \xi_2, \xi_3) := f(\xi_1 + \xi_2, \xi_3)f(\xi_2, \xi_3)^{-1} \\ \times f(\xi_1, \xi_2 + \xi_3)^{-1}f(\xi_1, \xi_2) \quad [4]$$

The group of 2-cocycles $Z^2(\Xi)$ consists of all 2-cochains f with $\partial f = 1$ and the group of all 2-coboundaries $B^2(\Xi)$ contains all 2-cochains of the form $f = \partial\varphi$. The 2-fold concatenation of the coboundary map is the trivial homomorphism $\partial \circ \partial = 1$, which implies that each 2-coboundary is a 2-cocycle. The converse is in general not the case and the 2-cohomology group $H^2(\Xi) := Z^2(\Xi)/B^2(\Xi)$ is nontrivial.

The Zmud (1971, 1972) analysis shows that the set of Weyl systems are characterized by elements of the 2-cohomology $H^2(\Xi)$. The multiplication of a Weyl system (w, f, \mathcal{H}) by a 1-cochain φ yields a new family of Weyl operators $(\varphi w)(\xi) = \varphi(\xi)w(\xi)$. The 2-cocycle f is altered by the multiplication of the 2-coboundary $\partial\varphi$ and the new Weyl system is given by $(\varphi w, \partial\varphi f, \mathcal{H})$. This kind of transformation does not change the cohomology class of the factor system and the corresponding Weyl algebras coincide: $\mathcal{A}(w, f, \mathcal{H}) = \mathcal{A}(\varphi w, \partial\varphi f, \mathcal{H})$. Thus, the fundamental properties of a Weyl system only depend on the cohomology class of the factor system. In particular, if the factor system $f = \partial\varphi$ is a 2-coboundary, then we can trivialize the Weyl system $(w, \partial\varphi, \mathcal{H})$ by multiplying the inverse 1-cochain φ^{-1} and we obtain a true unitary representation $(\varphi^{-1}w, 1, \mathcal{H})$. The corresponding Weyl algebra $\mathcal{A}(w, \partial\varphi, \mathcal{H})$ is abelian. The relation between cohomology and Weyl systems

can be made even more precise by the following theorem:

Theorem 1 (Zmud 1971, 1972). *θ is the group homomorphism on 2-cochains that exchanges the variables: $(\theta f)(\xi_1, \xi_2) = f(\xi_2, \xi_1)$.*

- (i) *The antisymmetric part $f^{-1}(\theta f)$ of a factor system (2-cocycle) is an antisymmetric bicharacter, that is, a group homomorphism in both arguments keeping the other variable fixed.*
- (ii) *Each symmetric 2-cocycle $f = \theta f$ is a 2-coboundary $f = \delta\varphi$.*
- (iii) *The group of antisymmetric bicharacters on Ξ is isomorphic to the 2-cohomology group $H^2(\Xi)$. For each antisymmetric bicharacter σ the corresponding 2-cohomology class is uniquely determined by $\sigma = f^{-1}(\theta f)$ for some representative $f \in Z^2(\Xi)$.*

Example 2 The following Weyl system describes n -quantum digits (in short qudits). The system's Hilbert space is spanned by orthonormal vectors $|a\rangle = |a_1, a_2, \dots, a_n\rangle$ which are labeled by vectors a of the additive group \mathbb{F}^n , where $\mathbb{F} = \mathbb{Z}_d$ is the cyclic field of prime order. A projective representation (w, χ, C^{d^n}) of the additive group \mathbb{F}^{2n} is given by

$$w(p, q)|a\rangle := e^{(2\pi i/d)p^t a}|a + q\rangle \quad [5]$$

where p^t is the transposed vector. The factor system χ assigns to each pair $(p, q), (p', q')$ the phase

$$\chi(p, q|p', q') := e^{(2\pi i/d)p^t q'} \quad [6]$$

The finite vector space \mathbb{F}^{2n} is interpreted as finite phase space with a multiplicative symplectic form σ . It assigns to a pair of vectors $(p, q), (a, b)$ the phase

$$\sigma(p, q|a, b) := e^{(2\pi i/d)(p^t b - a^t q)} \quad [7]$$

The commutation relation for Weyl operators comprise the symplectic form:

$$w(p, q)w(a, b) = \sigma(a, b|p, q)w(a, b)w(p, q) \quad [8]$$

The d^{2n} Weyl operators $w(p, q)$ are a basis of the algebra of all operators acting on the Hilbert space C^{d^n} , hence (w, χ, C^{d^n}) is irreducible. In particular, this Weyl system is a nice error basis in the sense of (Klappenecker and Roetteler 2002, 2005). Namely, the Weyl operators form a projective representation, on the one hand, and a unitary basis (Werner 2001) on the other.

For $d=2$ and $n=4$, we obtain a system of four qubits and the Weyl operators are tensor products of four Pauli matrices including the identity. For instance, the Weyl operator of the binary vector

$(p, q) = (0011, 1010)$ can be expressed in terms of Pauli matrices (see Introduction) as follows:

$$\begin{aligned} w(0011, 1010) &= w(0, 1) \otimes \mathbb{1} \otimes w(1, 1) \otimes w(1, 0) \\ &= iX \otimes \mathbb{1} \otimes Y \otimes Z \end{aligned} \quad [9]$$

Clifford Channels

Weyl systems can be seen as quantized symmetries corresponding to finite abelian groups. In the Heisenberg picture the symmetry transformations act on operators $A \in \mathcal{B}(\mathcal{H})$ of the observable algebra by automorphisms (reversible quantum channels):

$$\text{Ad}[w(\xi)](A) := w(\xi)Aw(\xi)^* \quad [10]$$

Since a projective representation preserves the group law up to a phase, the corresponding automorphisms preserve the group law:

$$\text{Ad}[w(\xi)] \circ \text{Ad}[w(\eta)] = \text{Ad}[w(\xi + \eta)] \quad [11]$$

A quantum channel T is called a Clifford channel if it is covariant with respect to Weyl systems $(w_1, f_1, \mathcal{H}_1)$ and $(w_2, f_2, \mathcal{H}_2)$, that is, the intertwining relation

$$T \circ \text{Ad}[w_2(\xi)] = \text{Ad}[w_1(\xi)] \circ T \quad [12]$$

holds. It is required that the antisymmetric part of the factor systems f_1 and f_2 coincide, that is, $\sigma = f_1^{-1}\theta f_1 = f_2^{-1}\theta f_2$. We call $(w_1, f_1, \mathcal{H}_1)$ the input and $(w_2, f_2, \mathcal{H}_2)$ the output system. We refer to the article by Scutaru (1979), which is concerned with the general properties of covariant channels.

It is a natural question to ask how Clifford channels act on Weyl operators. As shown by Holevo (n.d.), a Clifford channel maps Weyl operators of the output system to multiples of a Weyl operators of the input system, provided the input system is irreducible.

Theorem 3 (Holevo (n.d.)). *Let T be a Clifford channel such that the input system $(w_1, f_1, \mathcal{H}_1)$ is irreducible. Then there exists a function $\varphi: \Xi \rightarrow \mathbb{C}$ such that*

$$T(w_2(\xi)) = \varphi(\xi)w_1(\xi) \quad [13]$$

holds for all $\xi \in \Xi$. The function φ is of positive type, that is, for all complex functions f on Ξ the inequality

$$0 \leq \sum_{\xi, \eta \in \Xi} \varphi(\xi - \eta) \overline{f(\xi)} f(\eta) \quad [14]$$

holds. Conversely, if the factor systems $f_1 = f_2$ coincide, then a well-defined channel is determined

by [13] for any function φ of positive type with $\varphi(0) = 1$.

We apply Theorem 3 to a reversible Clifford channel T . Each output Weyl operator $w_2(\xi)$ is mapped to a multiple of an input Weyl operator

$$T(w_2(\xi)) = \varphi(\xi)w_1(\xi) \quad [15]$$

where φ is phase-valued (a 1-cochain) according to the reversibility of T . We focus now on the converse problem: construct all reversible Clifford channels for irreducible Weyl systems that have a common antisymmetric part of the factor system. The following theorem gives a useful characterization of reversible Clifford channels.

Theorem 4 (Schlingemann and Werner 2001). *If $(w_1, f_1, \mathcal{H}_1)$ and $(w_2, f_2, \mathcal{H}_2)$ are irreducible Weyl systems with $f_1^{-1}(\theta f_1) = f_2^{-1}(\theta f_2)$, then there exists a 1-cochain φ with coboundary $\delta\varphi = f_1^{-1}f_2$, and a reversible Clifford channel T_φ is determined by*

$$T_\varphi(w_2(\xi)) = \varphi(\xi)w_1(\xi) \quad [16]$$

If τ is a 1-cochain that also satisfies $\delta\tau = f_1^{-1}f_2$, then there exists $\eta \in \Xi$ such that

$$\tau(\xi) = \sigma(\eta|\xi)\varphi(\xi) \quad [17]$$

$$T_\tau = \text{Ad}[w_1(\eta)] \circ T_\varphi = T_\varphi \circ \text{Ad}[w_2(\eta)] \quad [18]$$

holds. In other words, two irreducible Weyl systems determine a reversible Clifford channel up to a “phase space translation η .”

We consider the Weyl system (w, f, \mathcal{H}) over a discrete phase space \mathbb{F}^{2n} , where \mathbb{F} is a finite field of prime order. The group of symplectic transformations $\text{Sp}(n, \mathbb{F})$ consists of all \mathbb{F} -linear maps s on the phase space \mathbb{F}^{2n} that preserve the symplectic form $\sigma = f^{-1}\theta f$. A further Weyl system $(w \circ s, f \circ s, \mathcal{H})$ is obtained for each symplectic transformation s . Here the factor system $f \circ s$ is defined according to $(f \circ s)(\xi, \eta) := f(s\xi, s\eta)$ and the corresponding Weyl operators are $(w \circ s)(\xi) = w(s\xi)$. Obviously, the antisymmetric part of the factor system $f \circ s$ is the symplectic form $\sigma \circ s = \sigma$. The following statement is a direct consequence of Theorem 4.

Corollary 5 *For each symplectic transformation $s \in \text{Sp}(n, \mathbb{F})$ there exists a 1-cochain φ with coboundary $\delta\varphi = f^{-1}(f \circ s)$ and the corresponding reversible Clifford channel $T_{[\varphi, s]}$ is given by*

$$T_{[\varphi, s]}(w(\xi)) = \varphi(\xi)w(s\xi) \quad [19]$$

with $\xi, \eta \in \mathbb{F}^{2n}$.

Example 6 We consider a finite field \mathbb{F} . To a symmetric matrix $\Gamma \in M_n(\mathbb{F})$ we associate the

symplectic transformation on \mathbb{F}^{2n} that maps a phase space vector (p, q) to $(p - \Gamma q, q)$. This shear transformation is viewed as one elementary step of a discrete dynamics. The quantized version of this dynamics is given by the unitary multiplication operator

$$u(\Gamma)|q\rangle = \zeta_d^{q^t \Gamma q}|q\rangle \quad [20]$$

with the root of unity $\zeta_d = \exp(i\pi(d+1)/d)$ for $d \neq 2$ and $\zeta_2 = i$. The unitary operator $u(\Gamma)$ implements a reversible Clifford operation for the symplectic transformation $(p, q) \mapsto (p - \Gamma q, q)$ since the relation

$$u(\Gamma)w(p, q)u(\Gamma)^* = \zeta_d^{q^t \Gamma q}w(p - \Gamma q, q) \quad [21]$$

holds. The symmetric matrix Γ describes a pattern of two-qudit interactions. This can be visualized by a graph Γ whose vertices are the positions $x, y = 1, \dots, n$. Two vertices x, y are connected by an edge if the matrix element $\Gamma_{xy}^x \neq 0$ is nonvanishing. The value of the matrix element Γ_{xy}^x is interpreted as the strength of the interaction.

Example 7 The second type of symplectic transformations, which is relevant here, is determined by an invertible matrix $C \in M_n(\mathbb{F})$. It induces a symplectic transformation which maps the vector (p, q) to $(Cq, -\tilde{C}p)$, where \tilde{C} is the inverse of the transpose of C . This is implemented by a unitary transformation $F_{[C]}$. It is called the Fourier transform associated with the invertible matrix C :

$$F_{[C]}|p\rangle = \frac{1}{\sqrt{d^n}} \sum_{q \in \mathbb{F}^n} e^{(2\pi i/d)p^t C q}|q\rangle \quad [22]$$

By construction, the relation

$$F_{[C]}w(p, q)F_{[C]}^* = e^{(2\pi i/d)p^t q}w(Cq, -\tilde{C}p) \quad [23]$$

follows. If $C = \text{diag}(c_1, \dots, c_n)$ is a diagonal matrix, then $F_{[C]}$ is a local unitary transformation. In fact, the Fourier transform is a tensor product

$$F_{[C]} = F_{[c_1]} \otimes F_{[c_2]} \otimes \dots \otimes F_{[c_n]} \quad [24]$$

with $c_x \in \mathbb{F} \setminus 0$, where the tensor product structure is determined by $|q\rangle = |q_1\rangle \otimes \dots \otimes |q_n\rangle$.

The Stabilizer Formalism

This section is dedicated to the stabilizer formalism, which has widely been discussed in the literature (Calderbank *et al.* 1997, Gottesman 1996, 1997). We investigated here stabilizer codes from a point of view of symmetries and show how they can be characterized by Clifford channels. We verify that

stabilizer codes are specific Clifford channels in the sense described in the last section. To begin with, we consider an irreducible Weyl system (w, f, \mathcal{H}) of an even-dimensional \mathbb{F} -vector space Ξ such that the antisymmetric part of the factor system $\sigma := f^{-1}\theta f$ is a symplectic form on Ξ . Furthermore, we need to introduce the following notions:

The symplectic complement of a subspace $Q \subset \Xi$ is the subspace

$$Q^\sigma = \{\xi \in \Xi \mid \sigma(\xi|q) = 1 \forall q \in Q\} \quad [25]$$

Furthermore, a subspace Q of Ξ is isotropic if it is contained in its symplectic complement $Q^\sigma \supset Q$. In other words, for all pairs of vectors $q, q' \in Q$ we have $\sigma(q|q') = 1$.

We consider an isotropic subspace Q and we denote by $(w|_Q, f|_Q, \mathcal{H})$ the corresponding restriction of the Weyl system (w, f, \mathcal{H}) . Since Q is isotropic, it follows that the restriction $f|_Q$ is symmetric. Hence, the Weyl algebra for the restricted system $\mathfrak{A}_Q := \mathfrak{A}(w|_Q, f|_Q, \mathcal{H})$ is an abelian subalgebra of $\mathcal{B}(\mathcal{H})$. As a consequence, all the operators in \mathfrak{A}_Q can be diagonalized simultaneously. To obtain the joint spectral resolution for all operators in A , we employ some facts from the theory of finite dimensional abelian C^* -algebras:

1. \mathfrak{A}_Q is a finite-dimensional abelian C^* -algebra and can be identified with the algebra of complex functions $\mathcal{C}(Q^\wedge)$ on a finite set Q^\wedge .
2. Each element $\varpi \in Q^\wedge$ is a character (pure state), that is, a linear functional such that $\varpi(AB) = \varpi(A)\varpi(B)$ and $\varpi(A^*) = \overline{\varpi(A)}$.
3. For each operator $A \in \mathfrak{A}_Q$ there exists precisely one function f_A on Q^\wedge which is uniquely determined by $\varpi(A) = f_A(\varpi)$. The isomorphism $A \rightarrow f_A$ is called the Gelfand isomorphism.
4. A character $\varpi \in Q^\wedge$ is an irreducible representation of \mathfrak{A}_Q and there is a unique projection e_ϖ onto the subspace in \mathcal{H} which carries this irreducible representation.

From these facts we derive a joint spectral resolution for all operators in \mathfrak{A}_Q . Namely, each $A \in \mathfrak{A}_Q$ can be written as

$$A = \sum_{\varpi \in Q^\wedge} e_\varpi \varpi(A) \quad [26]$$

We are now prepared to introduce the notion of stabilizer codes in accordance with Calderbank *et al.* (1997) and Gottesman (1996, 1997): Let Q be an isotropic subspace in Ξ and let $\varpi \in Q^\wedge$ be a character of \mathfrak{A}_Q . The projection e_ϖ is called a stabilizer code. The abelian group that is generated by the Weyl operators $w(q), q \in Q$, is called stabilizer group. The

abelian C^* -algebra \mathfrak{A}_Q is called stabilizer algebra. According to the following theorem, each stabilizer code is uniquely associated with a Clifford channel:

Theorem 8 (Schlingemann 2002, 2004). *Let Q be an isotropic subspace of Ξ and let e_ϖ be the stabilizer code of a character ϖ . Then there exists a unique Clifford channel E_ϖ with input system $(w_\varpi, f_\varpi, \mathcal{H}_\varpi)$ and output system $(w|_{Q^\sigma}, f|_{Q^\sigma}, \mathcal{H})$ such that the following is true:*

- (i) *For each $\xi \in \Xi$ the identity*

$$E_\varpi(w(\xi)) = \delta_{Q^\sigma}(\xi) w_\varpi(\xi) \quad [27]$$

is fulfilled.

- (ii) *Let $v_\varpi: \mathcal{H}_\varpi \rightarrow \mathcal{H}$ be the isometry which embeds \mathcal{H}_ϖ into \mathcal{H} , then*

$$E_\varpi(A) = v_\varpi^* A v_\varpi \quad [28]$$

holds for all $A \in \mathcal{B}(\mathcal{H})$.

- (iii) *The channel E_ϖ is invariant under translations in the isotropic subspace Q , that is, the identity*

$$E_\varpi \circ \text{Ad}[w(q)] = E_\varpi \quad [29]$$

holds for all $q \in Q$.

Stabilizer codes for maximally isotropic subspaces $Q = Q^\sigma$ are special, since the projection e_ϖ onto the eigenspace of the character ϖ is one-dimensional. Thus, e_ϖ is the density matrix of a pure state which is called stabilizer state. In view of Theorem 8, the expectation value of a Weyl operators $w(\xi)$ is given by

$$\text{tr}(e_\varpi w(\xi)) = \varpi(w(\xi)) \delta_Q(\xi) \quad [30]$$

Representation by Graphs

As described in the previous section (Theorem 8), each stabilizer codes is a pure Clifford channel which is completely determined by an isotropic subspace and a character of the corresponding stabilizer algebra. A constructive characterization of isotropic subspaces can be given in terms of graphs, as it has been shown in Schlingemann (2002, 2004). The complete description of a stabilizer code requires in addition the choice of a character of the stabilizer algebra. Both data, the isotropic subspace and the character, can be encoded in a single graph Λ . The set of vertices N is partitioned into four different types, the input vertices I , the output vertices J , the measurement vertices K and the syndrome vertices L (see Figure 1). The edges of the graph are undirected, and a pair of vertices can be connected by at most $d - 1$ edges, where self-links are also allowed. The adjacency matrix (also

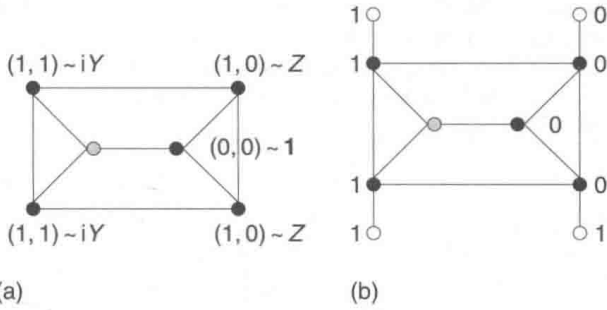


Figure 1 (a) A graphical representation of a Weyl operator $-Y \otimes Y \otimes Z \otimes Z \otimes 1$ of the stabilizer algebra of a quantum error correcting code, encoding one qubit into five (see 00273). The input vertex is gray, the output vertices are black. Each binary vector represents a Pauli matrix sitting at a tensor position of the output system. (b) The expectation values which are products over all edges, where to each edge with labels q, q' the value $(-1)^{qq'}$ is assigned. The character corresponds to the syndrome configuration (1110) (blanc vertices).

denoted by Λ) is a symmetric matrix with entries $\Lambda_{xy}^x = 0, 1, \dots, d-1$ according to the number of edges between x and y . Thus, the adjacency matrix can be seen as a linear operator on \mathbb{F}^N with cyclic field $\mathbb{F} = \mathbb{Z}_d$. Each subset $A \subset N$ corresponds to a linear projection onto the subspace $\mathbb{F}^A \subset \mathbb{F}^N$, which we denote by π_A . For a convenient description we introduce the following notation: the union of two sets of vertices is written without the symbol \cup , that is, instead of $I \cup J$ we write IJ .

Theorem 9 (Schlingemann 2002, 2004). *Let $Q \subset \mathbb{F}^J \oplus \mathbb{F}^J$ be an isotropic subspace and let ϖ be a character of the stabilizer algebra \mathcal{A}_Q . Then there exists a graph Λ with input vertices I , output vertices J , measurement vertices K and syndrome vertices L such that the following holds:*

- (i) *The linear operator $\pi_{JK} \Lambda \pi_{IKL}$ is invertible.*
- (ii) *The isotropic subspace Q consists of the vectors $(\pi_J \Lambda \pi_{JK} q, \pi_J q)$ with $q \in \ker(\pi_{IK} \Lambda \pi_{JK})$.*
- (iii) *There is a unique vector a in the syndrome subspace \mathbb{F}^L such that the expectation values of the character ϖ are given by*

$$\varpi(w(\pi_J \Lambda \pi_{JK} q, \pi_J q)) = \zeta_d^{(q+a)^t \Lambda(q+a)} \quad [31]$$

with $q \in \ker(\pi_{IK} \Lambda \pi_{JK})$.

Theorems 8 and 9 provide different useful characterizations of stabilizer codes, namely in terms of eigenspaces, Clifford channels, and graphs.

- The original definition of stabilizer codes in terms of eigenspaces goes back to Calderbank, Gottesman, Rains, Shor, and Sloane (see, e.g., Calderbank *et al.* (1997), Gottesman (1996, 1997)). They have developed an approach to derive quantum codes from classical binary codes.

- Stabilizer codes can also be characterized by specific Clifford channels (see Theorem 8). The condition for a channel to be a stabilizer code is the covariance with respect to a subgroup of phase space translations. This reflects stabilizer codes in terms of symmetries.
- Theorem 9 yields a characterization of stabilizer codes in terms of graphs providing an explicit expression for the isotropic subspace and the character of the stabilizer code. This graphical representation provides a suggestive encoding of various properties like error-correcting capabilities, multipartite entanglement, the effects of specific local operations. In fact, as it has been shown in Briegel and Raussendorf (2001), Dür *et al.* (2003), and Hein *et al.* (2004) that the entanglement present in a graph state can be derived from its shape.

See also: Capacities Enhanced by Entanglement; Quantum Error Correction and Fault Tolerance.

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Finitely Correlated States

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Introduction

A typical problem of quantum statistical mechanics is to compute equilibrium states of quantum dynamical systems. However, there is a strange difficulty inherent in this task, which is to describe the solution: if we try to describe the quantum state by specifying all matrix elements of all local density operators, we have a job which grows exponentially with the system size. This approach is obviously out of the question for the large systems statistical mechanics is interested in. Luckily, in practice nobody really wants to see all those numbers anyway, and one is content with determining a few correlation functions, or other easily parametrized characteristics of the state. But for computing a state in the first place, we cannot restrict the state description to a such parameters. So the problem there is again: how can we efficiently parametrize the states of interest?

In this article we collect some results on a particular way of addressing this problem. It originated in the early 1990s (Fannes *et al.* 1992b) in ideas for quantizing the notion of Markov chains (Accardi and Frigerio 1983). Recently, there has been a new surge of interest in such ideas, because they turned out to be very useful for numerical work on quantum spin chains.

Its typical feature is that one does not directly describe expectation values of the state, but instead generates the state from a description of its correlations between neighboring sites. In the language of quantum information theory, it could be said that the method focuses on the entanglement between different parts of the system.

The Basic Construction

Notation

We consider a quantum spin chain, that is, a system of infinitely subsystems, labeled by the integers, each

of which is a quantum-mechanical d -level system. Let us denote the observable algebra at site $x \in \mathbb{Z}$ by \mathcal{A}_x . Each \mathcal{A}_x is hence isomorphic to the $d \times d$ matrices. The observables of the whole (infinite) system lie in the infinite tensor product $\mathcal{A}_{\mathbb{Z}} = \bigotimes_{x \in \mathbb{Z}} \mathcal{A}_x$. This is defined as a quasilocal algebra (Bratteli and Robinson 1987, 1997), which is to say that it is the algebra generated by all finite tensor products of elements of the \mathcal{A}_x , say $\bigotimes_{x \in \Lambda} A_x$ with $A_x \in \mathcal{A}_x$ and Λ finite. Such an element is said to be localized in Λ , and we denote by \mathcal{A}_{Λ} the corresponding algebra. For $\Lambda_1 \subset \Lambda_2$, we identify \mathcal{A}_{Λ_1} with a subalgebra of \mathcal{A}_{Λ_2} , by tensoring with the identity operator on all sites in $\Lambda_2 \setminus \Lambda_1$. $\mathcal{A}_{\mathbb{Z}}$ is the completion of the union of all \mathcal{A}_{Λ} , with Λ finite, under the C^* -norm.

A state ω on $\mathcal{A}_{\mathbb{Z}}$ is uniquely specified by its expectations on the subalgebras \mathcal{A}_{Λ} . Since these are finite-dimensional matrix algebras, we can write $\omega(A) = \text{tr}(\rho_{\Lambda} A)$ for $A \in \mathcal{A}_{\Lambda}$, with a “local density operator” ρ_{Λ} . The system of local density operators must be consistent with respect to restrictions (partial traces).

So far we have not used the structure of the underlying lattice \mathbb{Z} in any way. This enters via the translation automorphisms τ_n of $\mathcal{A}_{\mathbb{Z}}$, which identify \mathcal{A}_x with \mathcal{A}_{x+n} . A state is called translationally invariant, if $\omega \circ \tau_n = \omega$. The translationally invariant states form a weakly compact convex subset of the state space of $\mathcal{A}_{\mathbb{Z}}$, whose extreme points are called ergodic states.

How to Generate Correlations

Correlations between parts of a systems typically have their origin in an interaction in the past. Even if the subsystems are dynamically separated later on, the correlation persists, and one can take this as a motivation to model correlations from two ingredients: a simplified prototype of a correlated system, and some evolution taking the parts of the simplified system to the parts of the given system. Let us consider a composite system, whose parts have observable algebras \mathcal{A}_1 and \mathcal{A}_2 , respectively, so that the whole system has algebra $\mathcal{A}_1 \otimes \mathcal{A}_2$. We can build a state ω on this system from a simpler one,

say a state η on some $\mathcal{B}_1 \otimes \mathcal{B}_2$, and two completely positive unit preserving maps $T_i: \mathcal{A}_i \rightarrow \mathcal{B}_i$ such that

$$\omega(A_1 \otimes A_2) = \eta(T_1(A_1) \otimes T_2(A_2))$$

Some features of η are inherited by ω . For example, when η is separable (a convex combination of products), which is always the case if either \mathcal{B}_1 or \mathcal{B}_2 is classical (i.e., an abelian algebra), then the same holds for ω . Hence, if we want to describe quantum correlated “entangled” states, we have to build the correlations on an entangled state η . Similarly, the “size” of the model system $\mathcal{B}_1 \otimes \mathcal{B}_2$ limits the strength of correlations in ω . As for every correlated state, we can look at the linear functionals on \mathcal{A}_2 , which are of the form $A \mapsto \omega(A_1 \otimes A)$ with fixed $A_1 \in \mathcal{A}_1$. The dimension of the space of such functionals might be called the correlation dimension of ω . This dimension is 1 for product states, and can clearly not increase by passing from η to ω . Hence, it is bounded by the dimensions of \mathcal{B}_1 and \mathcal{B}_2 , even if \mathcal{A}_1 and \mathcal{A}_2 are infinite dimensional. “Finite correlation” in the sense of the title of this article refers to the finiteness of the correlation dimension between the two halves of a spin chain.

The VBS Construction, and Matrix Product States

The so-called valence bond solid (VBS) states on a chain are constructed by applying these ideas to the correlations across every link of a spin chain. Let us introduce a correlated model state η_x on some algebra $\mathcal{B}_x^- \otimes \mathcal{B}_x^+$ for every bond $(x, x+1)$. Then the state at site x is a function of contributions from both bonds connecting it, and we express this by a completely positive map $T_x: \mathcal{A}_x \rightarrow \mathcal{B}_{x-1}^- \otimes \mathcal{B}_x^-$. Then an observable $A_1 \otimes \cdots \otimes A_L$ on a chain piece of length L is first mapped by $\bigotimes_{x=1}^L T_x$ to an element of $\mathcal{B}_0^+ \otimes \mathcal{B}_1^- \otimes \cdots \otimes \mathcal{B}_{L-1}^+ \otimes \mathcal{B}_L^-$. Evaluating with the states $\eta_1 \otimes \cdots \otimes \eta_{L-1}$, we are left with an element of $\mathcal{B}_0^+ \otimes \mathcal{B}_L^-$, which we can evaluate with yet another state η_{0L} describing the boundary conditions for the construction (see Figure 1).

Clearly, if we take the algebras \mathcal{B}_x^\pm large enough, and the model states η_x sufficiently highly entangled, we can generate every state on the finite chain. However, we can get an interesting class of states, even for fixed finite dimensions of the \mathcal{B}_x^\pm . By restricting this correlation dimension, we can set a level of complexity for the state description. We can then try to handle a given physical problem first with simple states of low correlation dimension, and increase this parameter only as needed. A typical problem here is to determine the ground state of a finite-range Hamiltonian. We can then optimize each T_x and η_x separately, minimizing the ground

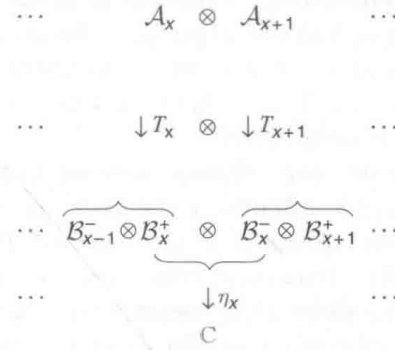


Figure 1

state energy with all other elements fixed. This is a semidefinite programming problem, for which very efficient methods are known. The global minimization is then done by letting the optimization site x sweep over the whole chain as often as needed.

In a ground-state problem one is looking for a pure state, and it is therefore sufficient to choose both the model states η_x and the operations T_x to pure, that is, without decomposition into sums of similar objects. The scheme is thus run at the vector level rather than the operator level: we take the algebras $\mathcal{B}_x^\pm = \mathcal{K}_x^\pm$ as the operators on a Hilbert space \mathcal{K}_x , and $\eta_x = (\dim \mathcal{K}_x)^{-1} |\Omega_x\rangle \langle \Omega_x|$ with the (unnormalized) maximally entangled vector

$$|\Omega_x\rangle = \sum_j |j\rangle \otimes |j\rangle \in \mathcal{K}_x \otimes \mathcal{K}_x \quad [1]$$

The maps T_x will be implemented by a single operator $V_x: \mathcal{K}_{x-1} \otimes \mathcal{K}_x \rightarrow \mathcal{H}$ as $T_x(A) = V_x^* A V_x$. Then the vectors $\Psi \in \mathcal{H}^{\otimes L}$ contributing to the state on the chain of length L are of the form

$$\begin{aligned} \Psi &= V_1 \otimes \cdots \otimes V_L (|j_0\rangle \otimes \Omega^{\otimes L} \otimes |j_L\rangle) \\ &= \sum_{j_0, j_1, \dots, j_L} (V_1 \otimes \cdots \otimes V_L) |j_0, j_1, j_1, \dots, j_{L-1}, j_L\rangle \end{aligned}$$

where j_0, j_L are labels for bases in \mathcal{K}_0 and \mathcal{K}_L , describing the possible choices at the boundary, and we have used the special form of Ω . We write out the operators V_x in components, so that

$$V_x |jj'\rangle = \sum_\mu |\mu\rangle V_{x;jj'}^\mu$$

with suitable $\dim \mathcal{K}_{x-1} \times \dim \mathcal{K}_x$ dimensional matrices V_x^μ , in terms of which the above expression can be interpreted as a matrix product. The components of Ψ in a product basis $\{|\mu\rangle\}$ become

$$\langle \mu_1, \dots, \mu_L | \Psi \rangle = \langle j_0 | V_1^{\mu_1} V_2^{\mu_2} \cdots V_L^{\mu_L} | j_L \rangle \quad [2]$$

Due to this form the states generated in this way have also been called “matrix product states” (Klümper 1991). If one wants to consider periodic

boundary conditions, the indices j_0 and j_L can also be contracted, and the expression becomes a trace. For some simulations it is also convenient to choose $\sim \mathcal{K}_0 = \dim \mathcal{K}_L = 1$, so there is only one matrix element to be considered.

The scheme for getting ground-state vectors described here is essentially the same as the density matrix renormalization group method (Verstraete *et al.* 2004). However, the version given here appears to be more transparent, more flexible, and in some cases (e.g., periodic boundary conditions) vastly more efficient. However, it may be too early for such judgment, since this is very much work in progress (Verstraete *et al.* 2005).

In the sequel, we will focus not so much on the numerical aspects, but on the possibility this construction offers to explicitly construct nontrivial translationally invariant states on the infinite chain. Numerically, even in a translation invariant situation the matrices V_x^μ obtained by optimization may turn out to depend on x (Wolf, Private Communication), that is, one has to admit the possibility of a spontaneous symmetry breaking. However, for the construction of states on the infinite chain we will simply fix all V_x to be equal. In some sense this turns the matrix product into a matrix power, which could be analyzed by methods familiar from the transfer matrix formalism of statistical mechanics. In eqn [2] this does not work, because of the μ -dependence of the matrices involved. Nevertheless, a slight reorganization of the construction will lead to a transfer-matrix-like formalism.

The Evolution Operator Construction

Fixing all T_x to be the same in Figure 1 still does not fix the state uniquely, since both in the mixed state version and in the pure state version of the construction some boundary information enters, as well. This boundary information then has to be chosen in such a way that a consistent family of local density operators is generated. It turns out that by rearranging the construction a little bit one can trivially solve one boundary condition, and reduce the other to finding a fixed point of a linear operator. This rearrangement was first carried out in Fannes *et al.* (1992b), where the term “finitely correlated state” was also coined.

The basic element of the VBS construction was the operators $T: \mathcal{A} \rightarrow \mathcal{B}^+ \otimes \mathcal{B}^-$ (here already taken independent of x). This is specified by $\dim \mathcal{A} \cdot \dim \mathcal{B}^+ \cdot \dim \mathcal{B}^-$ matrix elements. However, assuming we can identify the algebras \mathcal{B}^\pm , we can also consider these matrix elements as those of an “evolution operator” $E: \mathcal{A} \otimes \mathcal{B} \rightarrow \mathcal{B}$. This operator

is once again taken to be completely positive and unit preserving. We introduce its n th iterate $E^{(n)}: \mathcal{A}^{\otimes n} \otimes \mathcal{B} \rightarrow \mathcal{B}$ by the recursion

$$E^{(1)} = E, \quad E^{(n+1)} = E(\text{id}_{\mathcal{A}} \otimes E^{(n)}) \quad [3]$$

Clearly, these operators are again completely positive and unit preserving. Another way to express this iteration is to look at E as a family of maps on \mathcal{B} , parametrized by $A \in \mathcal{A}$: We set $E_A(B) = E(A \otimes B)$, and find

$$E^{(n)}(A_1 \otimes \cdots \otimes A_n \otimes B) = E_{A_1} \cdots E_{A_n}(B) \quad [4]$$

An important special role is played by the operator $\hat{E} = E_1$, which is again completely positive and unit preserving.

Now given any state η on \mathcal{B} , we get a state ω_n on $\mathcal{A}^{\otimes n}$, by setting

$$\omega_n(A_1 \otimes \cdots \otimes A_n) = \eta(E^{(n)}(A_1 \otimes \cdots \otimes A_n \otimes 1)) \quad [5]$$

Since $\hat{E}(1) = 1$, this family of states is consistent with respect to increasing n , by adding sites on the right, that is, $\omega_{n+1}(A \otimes 1) = \omega_n(A)$. In other words, the family ω_n defines a state on the infinite right half-chain. This state can be extended to the full chain, as a translationally invariant state if and only if consistency also holds for adding sites on the left, that is, if $\omega_{n+1}(1 \otimes A) = \omega_n(A)$ for all $A \in \mathcal{A}^{\otimes n}$. For this we need a condition on the state η : it must be invariant under the map \hat{E} (i.e., $\eta(\hat{E}(B)) = \eta(B)$ for all $B \in \mathcal{B}$). This is the only requirement, and we call ω the state \mathcal{A}_Z generated by E and η . Note that since \hat{E} has the invariant vector 1 , its transpose also has an invariant vector, which can also be chosen as a state. We will often look at unique invariant state, in which case we can call ω the state generated by E , without having to mention η .

The valence bond picture was very much suggested by trying to describe correlations in a spatially distributed quantum system (the chain). The construction given here is perhaps more readily suggested by a process in time, rather than space. In fact, the paper by Fannes *et al.* (1992b) was partly motivated by an attempt to define a quantum analog of Markov processes (Accardi and Frigerio 1983). In fact, we can think of the construction as a general form for a repeated measurement in quantum theory. The object on which the measurements are performed has observable algebra \mathcal{B} , whereas \mathcal{A} describes the successive outputs. Choosing \mathcal{A} to be classical (abelian) we would find in ω the joint probability distribution of the sequence of measured values, when the initial state of the object is η (not necessarily invariant). Allowing nonabelian \mathcal{A} would

then correspond to a family of delayed choice experiments: while \mathbb{E} describes the interaction of the system with the measurement apparatus (including the overall state change $\hat{\mathbb{E}}$), we are still free to make correlated and even entangled measurements on the successive output systems. This interpretation suggests many extensions, in particular, to continuous time (where the case of abelian outputs is discussed extensively in the classic book by Davies 1976), or to cases allowing an external quantum input in each step, in which case we are looking at a quantum channel with memory \mathcal{B} (Kretschmann and Werner 2005).

In spite of the different natural interpretations, however, the constructions in this and previous paragraphs give exactly the same class of translationally invariant states on the chain, as was shown in (Fannes *et al.* 1992b).

Ergodic Decomposition

A state on $\mathcal{A}_{\mathbb{Z}}$ is called ergodic if it is an extreme point of the compact convex subset of translationally invariant states. Often in statistical mechanics, one finds states which may be ergodic, but nevertheless contain a breaking of translation symmetry. Such states can be decomposed into periodic states, that is, states which are invariant with respect to some power of the shift. In general, new decompositions may become possible for any period. If no decomposition into periodic states is possible, the state is called completely ergodic.

In this section we consider the question of how to decompose a finitely correlated state into ergodic components, using a well-established connection between ergodicity and clustering properties (Bratteli and Robinson 1987, 1997), that is, the decay of correlation functions.

Correlation functions are very easily evaluated for finitely correlated states: let A_{\pm} be two observables localized on n_{\pm} sites, and suppose that these sites are separated by L sites. Then eqn [5] gives

$$\omega(A_- \otimes 1^{\otimes L} \otimes A_+) = \eta \left(E_{A_-}^{(n_-)} \hat{\mathbb{E}}^L E_{A_+}^{(n_+)}(1) \right) \quad [6]$$

The L -dependence of this operator is clearly governed by the matrix powers of $\hat{\mathbb{E}}$. By assumption this operator always has the eigenvalue 1, because $\hat{\mathbb{E}}(1)=1$, and has norm ≤ 1 , because it is also completely positive. The spectrum is hence contained in the unit circle. Each eigenvalue with modulus <1 thus contributes exponentially decaying terms to the correlation function [6]. From eigenvalues of modulus 1, which make up the so-called peripheral spectrum, we may get constant

or periodic contributions. This distinction is directly reflected in the ergodic properties (Fannes *et al.* 1992b):

- When the eigenvalue 1 is simple, there is a unique invariant state η , and $\lim_n n^{-1} \sum_{k=0}^{n-1} \hat{\mathbb{E}}^k(B) = \eta(B)1$. This implies, by [6] and (Bratteli and Robinson 1987, 1997, theorem 4.3.22), that ω is ergodic.
- When the eigenvalue 1 is simple, the peripheral spectrum consists precisely of the p th roots of unity for some $p \geq 1$. The state ω is then the equal-weight convex combination of p periodic states with period p , which are translates of each other.
- In particular (i.e., for $p=1$), a peripheral spectrum consisting only of the simple eigenvalue 1 implies that ω is exponentially clustering in the sense that

$$\begin{aligned} & |\omega(A_- \otimes 1^{\otimes L} \otimes A_+) - \omega(A_-)\omega(A_+)| \\ & \leq \text{poly}(L)r^L \|A_-\| \|A_+\| \end{aligned} \quad [7]$$

where r is the largest modulus of eigenvalues other than 1, and poly is polynomial obtained from the Jordan normal form of $\hat{\mathbb{E}}$. By the previous item, the state ω is then completely ergodic.

- Conversely, if a state is finitely correlated, and is ergodic (resp. completely ergodic), it has a representation such that 1 is a simple eigenvalue (resp. the peripheral spectrum is trivial).

Purity

Pure States

As in the case of the VBS construction, there is a version of the evolution operator construction, which is especially suited to produce pure states. Pure states are those which cannot be decomposed into a weighted sum of other states. For a translationally invariant state, this is a much stronger property than ergodicity and even complete ergodicity: not only the decomposition into periodic states is impossible, but any decomposition whatsoever. Nevertheless, this is what one expects from a ground state of translationally invariant interaction.

From the formula [5] it is clear that if we decompose the \mathbb{E} -operator entering for a site x into a sum two completely positive terms, we will have decomposed ω into two positive terms. These might still be equal, but it is certainly suggestive to look at states generated with an \mathbb{E} , which cannot be decomposed nontrivially into a sum of other

completely positive maps. Such maps are called pure, and are characterized by the form

$$\begin{aligned} \mathbb{E}(A \otimes B) &= V^*(A \otimes B)V \\ V : \mathbb{C}^k &\rightarrow \mathbb{C}^d \otimes \mathbb{C}^k \text{ is isometric} \end{aligned} \quad [8]$$

and \mathcal{A} and \mathcal{B} are the algebras of $d \times d$ and $k \times k$ matrices, respectively. Finitely correlated states generated from such a pure evolution operator are called purely generated. These are the candidates for pure finitely generated states.

The form of a pure map is reminiscent of the Stinespring dilation of a general completely positive map: for a general \mathbb{E} , we can set

$$\mathbb{E}(A \otimes B) = V^*(1_{\tilde{\mathcal{A}}} \otimes A \otimes B)V \quad [9]$$

where $\tilde{\mathcal{A}}$ is some auxiliary matrix algebra. Since the invariance condition for η does not involve the \mathcal{A} algebras, we get a purely generated state $\tilde{\omega}$ with one-site algebra $(\tilde{\mathcal{A}} \otimes \mathcal{A})$, whose restriction to the original chain is ω . Hence, purely generated states are the prototypes from which all other finitely correlated are obtained by sitewise restriction.

But are such states pure? Since $\hat{\mathbb{E}}$ need not have a trivial peripheral spectrum, the previous section tells us that a purely generated state may have a nontrivial decomposition into other, perhaps periodic states. But this is the only restriction we have to make. Indeed, the following statements about a finitely correlated state ω are equivalent (Fannes *et al.* 1994, theorem 1.5):

- ω is pure;
- ω is purely generated, and the operator $\hat{\mathbb{E}}$ has trivial peripheral spectrum;
- the mean entropy of ω vanishes, and ω is clustering, that is, [7] holds; and
- \mathbb{E} has the form [8], and no subalgebra of \mathcal{B} , which contains 1 , is invariant under all operators \mathbb{E}_A .

The Asymptotic Form of the Local Support

Let us now fix an isometry V , such that $\hat{\mathbb{E}}$ has trivial peripheral spectrum, and let ρ denote the unique invariant state of $\hat{\mathbb{E}}$. Then the vectors $\Psi \in \mathcal{H}^{\otimes n}$ in the support of ω are of the form [2] and depend, apart from the fixed choice of the $V_x^\mu \equiv V^\mu$, on the boundary indices $j_0, j_n = 1, \dots, k$. We can consider this as a map Γ_n from $k \times k$ matrices to $\mathcal{H}^{\otimes n}$:

$$\langle \mu_1, \dots, \mu_n | \Gamma_n(B) \rangle = \text{tr}(BV^{\mu_1} V^{\mu_2} \dots V^{\mu_n}) \quad [10]$$

and denote the range of Γ_n by \mathcal{G}_n . Then \mathcal{G}_n is at most k^2 -dimensional. Moreover, this family of subspaces is nested, that is, $\mathcal{G}_{n+m} \subseteq \mathcal{G}_n \otimes \mathcal{H}^{\otimes m}$ and $\mathcal{G}_{n+m} \subseteq \mathcal{H}^{\otimes m} \otimes \mathcal{G}_m$. Using that $\hat{\mathbb{E}}(B)^n \rightarrow \rho(B)1$ converges exponentially fast, we also find that Γ_n is asymptotically an isometry between \mathcal{G}_n and the Hilbert

space of $k \times k$ matrices with scalar product $\langle B, C \rangle_\rho = \text{tr}(\rho B^* C)$. Hence, all the spaces \mathcal{G}_n are asymptotically identified, even though they are contained in each other. This “self-similarity” is the source of many further properties. For example, for any density matrix $\tilde{\rho}$ on $\ell + m + r$ sites supported by $\mathcal{G}_{\ell+m+r}$, and any observable A , localized on m sites in the middle of this interval (with ℓ to the left and r to the right), we get the expectation $\text{tr}(\tilde{\rho} A) \approx \omega(A)$, up to exponentially small terms depending only on ℓ and r .

Ground States and Gaps

Suppose we fix some interval length ℓ , and let h be the projection onto the complement of \mathcal{G}_ℓ in $\mathcal{H}^{\otimes \ell}$. We now consider h as the interaction term of a lattice interaction, that is, we consider the formal Hamiltonian

$$H = \sum_x \tau_x(h) \quad [11]$$

Then in the finitely correlated state ω , each term in this sum has expectation zero, which is the absolute minimum for such expectations, because $h \geq 0$. In this sense ω is the ground state for this Hamiltonian. Usually, ground states are not characterized in this way: one can only require that the average energy is minimized with respect to all translationally invariant states (Bratteli and Robinson 1987, 1997, theorem 6.2.58). Hence, one can usually perturb a ground state locally such that some terms in [11] have less than average expectation, at the expense of others. For ω this is clearly impossible. Moreover, any state ω' with $\omega'(\tau_x(h)) = 0$ for all x must coincide with ω , even if we do not impose translation invariance. This follows from the previous section: the local density operators of ω' must all be supported in \mathcal{G}_n by the nesting property; hence, if we compare density operators on intervals of length $\ell + m + r$ on observables localized on the middle m sites, we get $\omega'(A) \approx \omega(A)$, up to errors exponentially small in ℓ and r .

The Hamiltonian [11] involves an infinite sum, which can be mathematically understood as a quadratic form in the GNS-representation associated with ω (Bratteli and Robinson 1987, 1997). This is the Hilbert space spanned by vectors written as $A\Omega$, with the scalar products $\langle A\Omega, B\Omega \rangle = \omega(A^* B)$, for local operators A, B . The ground-state property then implies $H\Omega = 0$, and $H \geq 0$, because $h \geq 0$. It can be seen that H generates a well-defined dynamics, and is essentially self-adjoint on the domain of such vectors. Thus also the spectrum of H is a well-defined concept. This suggests a strengthening of the

ground-state property: not only is Ω the unique eigenvector of H for eigenvalue 0, but there is a gap $\gamma > 0$ between zero and the next eigenvalue. This property is of considerable interest for models in solid-state physics and statistical mechanics. It was shown for all ergodic pure finitely correlated states in (Fannes *et al.* 1992b).

Density

Density of Finitely Correlated Pure States

The natural topology in which to consider the approximation between states on the chain is the weak topology. A sequence ω_n converges weakly to ω if for all local A the expectations converge, that is, $\omega_n(A) \rightarrow \omega(A)$.

Let us start from an arbitrary translationally invariant state ω , and see how we can approximate it. First, we can split the chains into intervals of length L , and replace ω by the tensor product of the restrictions of ω to each of these intervals. This state is not translationally invariant, so we average it over the L translations, and call the resulting state ω_L . Consider a local observable A , whose localization region has length R . Then for $L - R$ out of the L translates contributing to ω_L the expectation will be the same as for ω , and we get

$$\omega_L(A) = \left(1 - \frac{R}{L}\right)\omega(A) + \frac{R}{L}\tilde{\omega}(A),$$

where the error term $\tilde{\omega}$ is again a state. Hence, ω_L converges weakly to ω as $L \rightarrow \infty$. One can show easily that ω_L is finitely correlated, with an algebra \mathcal{B} essentially equal to $\mathcal{A}^{\otimes L}$. Hence, the finitely correlated states are weakly dense in the set of translationally invariant states.

We can make the approximating states purer by a very simple trick. In the previous construction we always take two intervals together, and replace the tensor product of the two restrictions by a purification, that is, by a pure state on an interval of length $2L$, whose restrictions to the two length- L subintervals coincide with ω . We average this over $2L$ translates, and call the result η_L . The estimates showing that $\eta_L \rightarrow \omega$ weakly are exactly the same as before. Moreover, one can show (Fannes *et al.* 1992a) that η_L is purely generated.

Being defined as a convex combination of other states, η_L is not pure, and the peripheral spectrum of \hat{E} will contain all the $2L$ th roots of unity. However, we can use that such a rich peripheral spectrum is not generic for \hat{E} constructed from an isometry V . Therefore, if we choose an isometry V_ϵ close to the isometry V generating η_L , we obtain a purely

generated state η_L^ϵ with trivial peripheral spectrum. Since the expression for expectations of such states depends continuously on the generating isometry, we have that $\eta_L^\epsilon \rightarrow \eta_L$ as $\epsilon \rightarrow 0$. But we know from the previous section that such states are pure. Hence, the pure finitely correlated states are weakly dense in the set of all translationally invariant states (Fannes *et al.* 1992a).

This has implications for the geometry of the compact convex set of translationally invariant states, which are rather counter-intuitive for the intuitions trained on finite-dimensional convex bodies. To begin with, the extreme points (the ergodic states) are dense in the whole body. This is not such a rare occurrence in infinite-dimensional convex sets, and is shared, for example, by the set of operators F with $0 \leq F \leq 1$ on an infinite-dimensional Hilbert space (Davies 1976). Together with the property that the translationally invariant states form a simplex, it actually fixes the structure of this compact convex set to be the so-called Poulsen simplex. This was known also without looking at finitely correlated states. The rather surprising result of the above density argument is that even the small subclass of states which are extremal, not only in the translationally invariant subset but even in the whole state space, is still dense.

Finitely Correlated Pure States with Bounded Memory Dimension

It is clear in the above construction that the dimension of the algebra \mathcal{B} goes to infinity for an approximating sequence. How many states can we get with a fixed memory algebra \mathcal{B} ? The dimension of this manifold can be estimated easily from the number of parameters needed to describe the map E , and this dimension is certainly small compared to the dimension of the state space of the length L piece of the chain as $L \rightarrow \infty$. However, since this is an infinite set, and not a linear subspace, we do not get an immediate bound on the dimension of the linear span of these states. What we want to show in this section is that the space of finitely correlated states with fixed \mathcal{B} nevertheless generates a low-dimensional subspace of states on any large interval of the chain. To this end we will have to exhibit many observables A , localized on L sites, whose expectation is the same for all finitely correlated states with given \mathcal{B} .

Let us look first at the case of purely generated states, or rather at the vectors $\Psi \in \mathcal{H}^{\otimes L}$, which can be written in the form [2], which in the translation invariant case becomes

$$\langle \mu_1, \dots, \mu_L | \Psi \rangle = \langle j_0 | V^{\mu_1} V^{\mu_2} \dots V^{\mu_L} | j_L \rangle \quad [12]$$

for some collection V^1, \dots, V^d of $k \times k$ matrices, and some basis labels $j_0, j_L \in \{1, \dots, k\}$. The span of all such vectors will be denoted by $\mathcal{V}_L(k, d)$, and we would like to analyze the growth of $\dim \mathcal{V}_L(k, d)$, as $L \rightarrow \infty$. Now a vector with components $a(\mu_1, \dots, \mu_L)$ lies in the orthogonal complement of $\mathcal{V}_L(k, d)$ if and only if

$$\sum_{\mu_1, \dots, \mu_L} a(\mu_1, \dots, \mu_L) V^{\mu_1} V^{\mu_2} \dots V^{\mu_L} = 0$$

for any collection of matrices V^μ . In other words, this expression, considered as a noncommutative polynomial in d variables, is a polynomial identity for $k \times k$ matrices. The simplest such identity, for $k=2$, $d=3$, $L=5$, is $[A, [B, C]^2] = 0$. (For the proof observe that $[B, C]$ is traceless, so its square is a multiple of the identity by the Cayley–Hamilton theorem.) This identity alone implies the existence of many more identities. For example, we can substitute higher-order polynomials for A, B, C , and multiply the identity with arbitrary polynomial from the right or from the left. There is a well-developed theory for such identities, called the theory of polynomial identity (PI) rings. In that context, the precise growth we are looking for has been worked out (Drensky 1998):

$$\lim_{L \rightarrow \infty} \frac{\log \dim \mathcal{V}_L(k, d)}{\log L} = (d-1)k^2 + 1 \quad [13]$$

Thus, the $\dim \mathcal{V}_L(k, d)$ only grows like a polynomial in L , of known degree, and the joint support of all purely generated finitely correlated state is exponentially small compared to $\mathcal{H}^{\otimes L}$.

We can apply the same idea to the set of all finitely correlated states with \mathcal{B} equal to the $k \times k$ matrices. The joint support in this case is the full space, since the trace state on the chain, which is a product state generated with $k=1$, already has full support. However, it is still true all but a polynomial number of expectation values of ω are already fixed by specifying k . Indeed, formula [5] for a general state is precisely of

the form [12], with the difference that the arguments A replace μ , and the matrices \mathbb{E}_A are now operators on the k^2 -dimensional space \mathcal{B} . If we only want an upper bound, we can ignore sublattices coming from Hermiticity and normalization constraints on \mathbb{E} , and we get that the dimension of all finitely correlated states generated from the $k \times k$ matrices, restricted to a subchain of length L , grows at most like L^α , with $\alpha \leq (d^2 - 1)k^2 + 1$.

See also: Ergodic Theory; Quantum Spin Systems; Quantum Statistical Mechanics: Overview.

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Finite-Type Invariants

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Introduction

Knots belong to sailors and climbers and upon further reflection, perhaps also to geometers, topologists, or combinatorialists. Surprisingly, throughout the 1980s,

it became apparent that knots are also closely related to several other branches of mathematics in general and mathematical physics in particular. Many of these connections (though not all!) factor through the notion of “finite-type invariants” (aka “Vassiliev” or “Goussarov–Vassiliev” invariants) (Goussarov 1991, 1993, Vassiliev 1990, 1992, Birman–Lin 1993, Kontsevich 1993, Bar-Natan 1995).

Let V be an arbitrary invariant of oriented knots in oriented space with values in some abelian group A . Extend V to be an invariant of 1-singular knots, knots

that may have a single singularity that locally looks like a double point \times , using the formula

$$V(\times) = V(\times) - V(\times) \quad [1]$$

Further extend V to the set \mathcal{K}^m of m -singular knots (knots with m double points) by repeatedly using [1].

Definition 1 We say that V is of type m if its extension $V|_{\mathcal{K}^{m+1}}$ to $(m+1)$ -singular knots vanishes identically. We also say that V is of finite type if it is of type m for some m .

Repeated differences are similar to repeated derivatives; hence, it is fair to think of the definition of $V|_{\mathcal{K}^m}$ as repeated differentiation. With this in mind, the above definition imitates the definition of polynomials of degree m . Hence, finite-type invariants can be considered as “polynomials” on the space of knots.

As described in the section “Basic facts”, finite-type invariants are plenty and powerful and they carry a rich algebraic structure and are deeply related to Lie algebras. There are several constructions for a “universal finite-type invariant” and those are related to conformal field theory, the Chern–Simons–Witten topological quantum field theory, and Drinfel’d’s theory of associators and quasi-Hopf algebras (see the section “The proofs of the fundamental theorem”). Finite-type invariants have been studied extensively (see the section “Some further directions”) and generalized in several directions (see the section “Beyond knots”). But the first question on finite-type invariants remains unanswered:

Problem 2 *Honest polynomials are dense in the space of functions. Are finite-type invariants dense within the space of all knot invariants? Do they separate knots?*

In a similar way, one may define finite-type invariants of framed knots (and ask the same questions).

Basic Facts

Classical Knot Polynomials

The first (nontrivial!) thing to notice is that there are plenty of finite-type invariants and they are at least as powerful as all the standard knot polynomials combined (finite-type invariants are like polynomials on the space of knots; the standard phrase “knot polynomials” refers to a different thing – knot invariants with polynomial values):

Theorem 3 (Bar-Natan 1995, Birman-Lin 1993). *Let $J(K)(q)$ be the Jones polynomial of a knot K (it is a Laurent polynomial in a variable q). Consider the*

power series expansion $J(K)(e^x) = \sum_{m=0}^{\infty} V_m(K)x^m$. Then each coefficient $V_m(K)$ is a finite-type knot invariant (thus, the Jones polynomial can be reconstructed from finite-type information).

A similar theorem holds for the Alexander–Conway, HOMFLY-PT, and Kauffman polynomials (Bar-Natan 1995), and indeed, for arbitrary Reshetikhin–Turaev invariants (Reshetikhin and Turaev 1990, Lin 1991), although it is still unknown if the signature of a knot can be expressed in terms of its finite-type invariants.

Chord Diagrams and the Fundamental Theorem

The top derivatives of a multivariable polynomial form a system of constants which determine the polynomial up to polynomials of lower degree. Likewise the m th derivative $V^{(m)} := V(\times^m \cdot \times)$ of a type m invariant V is a constant (for $V(\times^m \cdot \times \times \times) - V(\times^m \cdot \times \times \times) = V(\times^{m+1} \times) = 0$ so $V^{(m)}$ is blind to 3D topology), and likewise $V^{(m)}$ determines V up to invariants of lower type. Hence, a primary tool in the study of finite-type invariants is the study of the “top derivative” $V^{(m)}$, also known as “the weight system of V .”

Blind to 3D topology, $V^{(m)}$ only sees the combinatorics of the circle that parametrizes an m -singular knot. On this circle, there are m pairs of points that are pairwise identified in the image; one indicates those by drawing a circle with m chords marked (an “ m -chord diagram”) (see Figure 1).

Definition 4 Let \mathcal{D}_m denote the space of all formal linear combinations with rational coefficients of m -chord diagrams. Let \mathcal{A}_m^r be the quotient of \mathcal{D}_m by all 4T and FI relations as drawn in Figure 2 (full details are given in, e.g., Bar-Natan (1995)), and let $\hat{\mathcal{A}}^r$ be the graded completion of $\mathcal{A} := \bigoplus_m \mathcal{A}_m^r$. Let $\mathcal{A}_m, \mathcal{A}$, and $\hat{\mathcal{A}}$ be the same as $\mathcal{A}_m^r, \mathcal{A}^r$, and $\hat{\mathcal{A}}^r$ but without imposing the FI relations.

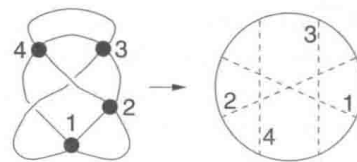


Figure 1 A 4-singular knot and its corresponding chord diagram.



Figure 2 The 4T and FI relations.

Theorem 5 (The fundamental theorem)

- (Easy part). If V is a rational valued type m -invariant then $V^{(m)}$ defines a linear functional on \mathcal{A}_m^r . If in addition $V^{(m)} \equiv 0$, then V is of type $m - 1$.
- (Hard part). For any linear functional W on \mathcal{A}_m^r , there is a rational valued type m invariant V so that $V^{(m)} = W$.

Thus, to a large extent, the study of finite-type invariants is reduced to the finite (though super-exponential in m) algebraic study of \mathcal{A}_m^r . A similar theorem reduces the study of finite-type invariants of framed knots to the study of \mathcal{A}_m .

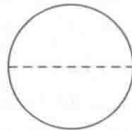
The Structure of \mathcal{A}

Knots can be multiplied (the “connected sum” operation) and knot invariants can be multiplied. This structure interacts well with finite-type invariants and induces the following structure on \mathcal{A}^r and \mathcal{A} :

Theorem 6 (Kontsevich 1993, Bar-Natan 1995, Willerton 1996, Chmutov et al. 1994). \mathcal{A}^r and \mathcal{A} are commutative and cocommutative graded bialgebras (i.e., each carries a commutative product and a compatible cocommutative coproduct). Thus, both \mathcal{A}^r and \mathcal{A} are graded polynomial algebras over their spaces of primitives, $\mathcal{P}^r = \bigoplus_m \mathcal{P}_m^r$ and $\mathcal{P} = \bigoplus_m \mathcal{P}_m$.

Framed knots differ from knots only by a single integer parameter (the “self-linking,” itself a type 1 invariant). Thus, \mathcal{P}^r and \mathcal{P} are also closely related.

Theorem 7 (Bar-Natan 1995). $\mathcal{P} = \mathcal{P}^r \oplus \langle \theta \rangle$, where θ is the unique 1-chord diagram:



Bounds and Computational Results

Table 1 shows the number of type m -invariants of knots and framed knots modulo type $m - 1$ invariants ($\dim \mathcal{A}_m^r$ and $\dim \mathcal{A}_m$) and the number of multiplicative generators of the algebra \mathcal{A} in degree m ($\dim \mathcal{P}_m$) for $m \leq 12$. Some further tabulated results are in Bar-Natan (1996).

Table 1 Some dimensions of spaces of finite type invariants

m	0	1	2	3	4	5	6	7	8	9	10	11	12
$\dim \mathcal{A}_m^r$	1	0	1	1	3	4	9	14	27	44	80	132	232
$\dim \mathcal{A}_m$	1	1	2	3	6	10	19	33	60	104	184	316	548
$\dim \mathcal{P}_m$	0	1	1	1	2	3	5	8	12	18	27	39	55

Source: Bar-Natan (1995); Kneissler (1997).

Little is known about these dimensions for large m . There is an explicit conjecture in Broadhurst (1997), but no progress has been made in the direction of proving or disproving it. The best asymptotic bounds available are the following.

Theorem 8 For large m , $\dim \mathcal{P}_m > e^{c\sqrt{m}}$ (for any fixed $c < \pi\sqrt{2/3}$) and $\dim \mathcal{A}_m < 6^m m! \sqrt{m} / \pi^{2m}$ (Stoimenow 1998, Zagier 2001).

Jacobi Diagrams and the Relation with Lie Algebras

Much of the richness of finite-type invariants stems from their relationship with Lie algebras. Theorem 9 below suggests this relationship on an abstract level, Theorem 10 makes that relationship concrete, and Theorem 12 makes it a bit deeper.

Theorem 9 (Bar-Natan 1995). The algebra \mathcal{A} is isomorphic to the algebra \mathcal{A}^t generated by “Jacobi diagrams in a circle” (chord diagrams that are also allowed to have oriented internal trivalent vertices) modulo the AS, STU, and IHX relations (see Figure 3).

Thinking of trivalent vertices as graphical analogs of the Lie bracket, the AS relation becomes the anti-commutativity of the bracket, STU becomes the equation $[x, y] = xy - yx$, and IHX becomes the Jacobi identity. This analogy is made concrete within the proof of the following:

Theorem 10 (Bar-Natan 1995). Given a finite-dimensional metrized Lie algebra \mathfrak{g} (e.g., any semi-simple Lie algebra), there is a map $T_{\mathfrak{g}}: \mathcal{A} \rightarrow \mathcal{U}(\mathfrak{g})^{\mathfrak{g}}$ defined on \mathcal{A} and taking values in the invariant part $\mathcal{U}(\mathfrak{g})^{\mathfrak{g}}$ of the universal enveloping algebra $\mathcal{U}(\mathfrak{g})$ of \mathfrak{g} . Given also a finite-dimensional representation R of \mathfrak{g} there is a linear functional $W_{\mathfrak{g}, R}: \mathcal{A} \rightarrow \mathbb{Q}$.

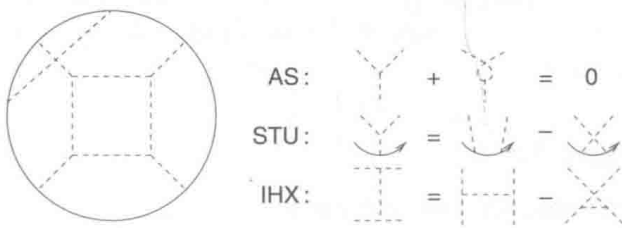


Figure 3 A Jacobi diagram in a circle and the AS, STU, and IHX relations.

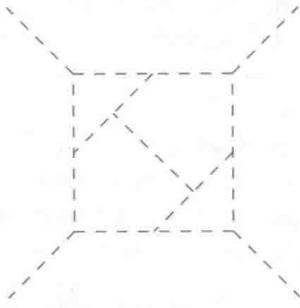


Figure 4 A free Jacobi diagram.

The last assertion along with Theorem 5 show that associated with any \mathfrak{g} , R , and m , there is a weight system and hence a knot invariant. Thus, knots are unexpectedly linked with Lie algebras.

The hope (Bar-Natan 1995) that all finite-type invariants arise in this way was dashed by Vogel (1997, 1999) and Lieberum (1999). But finite-type invariants that do not arise in this way remain rare and not well understood.

The Poincaré–Birkhoff–Witt (PBW) theorem of the theory of Lie algebras says that the obvious “symmetrization” map $\chi_{\mathfrak{g}}: \mathcal{S}(\mathfrak{g}) \rightarrow \mathcal{U}(\mathfrak{g})$ from the symmetric algebra $\mathcal{S}(\mathfrak{g})$ of a Lie algebra \mathfrak{g} to its universal enveloping algebra $\mathcal{U}(\mathfrak{g})$ is a \mathfrak{g} -module isomorphism. The following definition and theorem form a diagrammatic counterpart of this theorem:

Definition 11 Let \mathcal{B} be the space of formal linear combinations of “free Jacobi diagrams” (Jacobi diagrams as before, but with unmarked univalent ends (“legs”) replacing the circle; see an example in Figure 4), modulo the AS and IHX relations of before. Let $\chi: \mathcal{B} \rightarrow \mathcal{A}$ be the symmetrization map which maps a k -legged free Jacobi diagram to the average of the $k!$ ways of planting these legs along a circle.

Theorem 12 (Diagrammatic PBW; Kontsevich 1993, Bar-Natan 1995). χ is an isomorphism of vector spaces. Furthermore, fixing a metrized \mathfrak{g} there is a commutative square as in Figure 5.

Note that \mathcal{B} can be graded (by half the number of vertices in a Jacobi diagram) and that χ respects

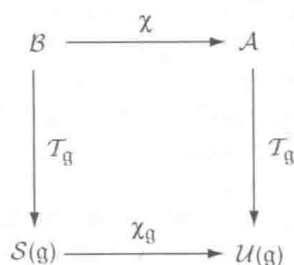


Figure 5 The diagrammatic PBW isomorphism and its classical counterpart.

degrees so it extends to an isomorphism $\chi: \hat{\mathcal{B}} \rightarrow \hat{\mathcal{A}}$ of graded completions.

Proofs of the Fundamental Theorem

The heart of all known proofs of Theorem 5 is always a construction of a “universal finite-type invariant” (see below); it is simple to show that the existence of a universal finite-type invariant is equivalent to Theorem 5.

Definition 13 A universal finite-type invariant is a map $Z: \{\text{knots}\} \rightarrow \hat{\mathcal{A}}'$ whose extension to singular knots satisfies $Z(K) = D + (\text{higher degrees})$ whenever a singular knot K and a chord diagram D are related as discussed before.

The Kontsevich Integral

The first construction of a universal finite-type invariant was given by Kontsevich (1993) (see also Bar-Natan (1995) and Chmutov and Duzhin (2001)). It is known as “the Kontsevich integral” and up to a normalization factor it is given by

$$Z_1(K) = \sum_{m=0}^{\infty} \frac{1}{(2\pi i)^m} \sum_{\substack{t_1 < \dots < t_m \\ P = \{(z_i, z'_i)\}}} (-1)^{\#P_1} D_P \bigwedge_{i=1}^m \frac{dz_i - dz'_i}{z_i - z'_i}$$

where the relationship between the knot K , the pairing P , the real variables t_i , the complex variables z_i and z'_i , and the chord diagram D_P is summarized in Figure 6 (the symbol \sum means “sum over all discrete variables and integrate over all continuous variables.”)

The Kontsevich integral arises from studying the holonomy of the Knizhnik–Zamolodchikov equation of conformal field theory (Knizhnik and Zamolodchikov 1984). When evaluating Z_1 , one encounters multiple ζ -numbers (Le-Murakami 1995) in a substantial way, and the proof that the end result is rational is quite involved (Le-Murakami 1996) and relies on deep results about associators and quasitriangular quasi-Hopf algebras (Drinfel’d 1990, 1991). Employing the same techniques, in Le-Murakami

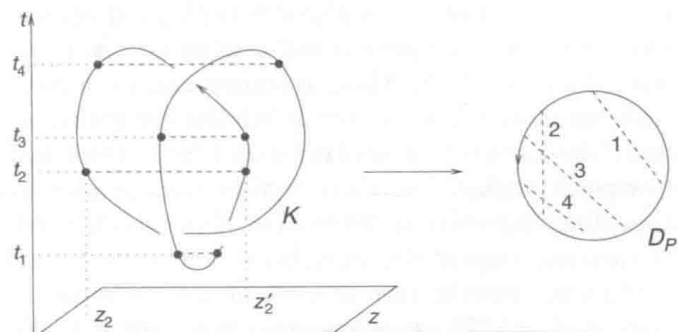


Figure 6 The key ingredients of the Kontsevich integral.

(1996), it is also shown that the composition of $W_{g,R} \circ Z_1$ precisely reproduces the Reshetikhin–Turaev invariants (Reshetikhin and Turaev 1990).

Perturbative Chern–Simons–Witten Theory and Configuration Space Integrals

Historically, the first approach to the construction of a universal finite-type invariant was to use perturbation theory with the Chern–Simons–Witten topological quantum field theory; this is also how the relationship with Lie algebras first arose. But taming the integrals involved turned out to be difficult and working constructions using this approach appeared only a bit later.

In short, one writes a perturbative expansion for the large k asymptotics of the Chern–Simons–Witten path integral for some metrized Lie algebra \mathfrak{g} with a Wilson loop in some representation R of \mathfrak{g} ,

$$\int_{\mathfrak{g}\text{-connections}} \mathcal{D}A \operatorname{tr}_R \operatorname{hol}_K(A) \times \exp \left[\frac{ik}{4\pi} \int_{\mathbb{R}^3} \operatorname{tr} \left(A \wedge dA + \frac{2}{3} A \wedge A \wedge A \right) \right]$$

The result is of the form

$$\sum_{D: \text{Feynman diagram}} W_{\mathfrak{g}(D),R} \oint \mathcal{E}(D)$$

where $\mathcal{E}(D)$ is a very messy integral expression and the diagrams D as well as the weights $W_{\mathfrak{g}(D),R}$ were already discussed before. Replacing $W_{\mathfrak{g}(D),R}$ by simply D in the above formula, we get an expression with values in $\hat{\mathcal{A}}$:

$$Z_2(K) := \sum_D D \oint \mathcal{E}(D) \in \hat{\mathcal{A}}$$

For formal reasons $Z_2(K)$ ought to be a universal finite-type invariant, and after much work taming the $\mathcal{E}(D)$ factors and after multiplying by a further framing-dependent renormalization term Z^{anomaly} , the result is indeed a universal finite-type invariant.

Upon further inspection, the $\mathcal{E}(D)$ factors can be reinterpreted as integrals of certain spherical volume forms on certain (compactified) configuration spaces (Bott–Taubes 1994). These integrals can be further interpreted as counting certain “tinker toy constructions” built on top of K (Thurston 1995). The latter viewpoint makes the construction of Z_2 visually appealing (Bar-Natan 2000), but there is no satisfactory write-up of this perspective yet.

We note that the precise form of the renormalization term Z^{anomaly} remains an open problem. An appealing conjecture is that $Z^{\text{anomaly}} = \exp(1/2)\omega$. If

this is true then $Z_2 = Z_1$ (Poirier 1999); but the conjecture is only verified up to degree 6 (Lescop 2001) (there is also an unconfirmed verification to all orders (Yang 1997)).

The most important open problem about perturbative Chern–Simons–Witten theory is not directly about finite-type invariants, but it is nevertheless worthwhile to recall it here:

Problem 14 *Does the perturbative expansion of the Chern–Simons–Witten theory converge (or is asymptotic to) the exact solution due to Witten (1989) and Reshetikhin and Turaev (1990) when the parameter k converges to infinity?*

Associators and Trivalent Graphs

There is also an entirely algebraic approach for the construction of a universal finite-type invariant Z_3 . The idea is to find some algebraic context within which knot theory is finitely presented – that is, presented by finitely many generators subject to finitely many relations. If the algebraic context at hand is compatible with the definitions of finite-type invariants and of chord diagrams, one may hope to define Z_3 by defining it on the generators in such a way that the relations are satisfied. Thus, the problem of defining Z_3 is reduced to finding finitely many elements of \mathcal{A} -like spaces which solve certain finitely many equations.

A concrete realization of this idea is in Le-Murakami (1996) and Bar-Natan (1997) (following ideas from Drinfel’d (1990, 1991) on quasitriangular quasi-Hopf algebras). The relevant “algebraic context” is a category with certain extra operations, and within it, knot theory is generated by just two elements, the braiding \bowtie and the re-association \wr . Thus, to define Z_3 it is enough to find $R = Z_3(\bowtie)$ and “an associator” $\Phi = Z_3(\wr)$ which satisfy certain normalization conditions as well as the pentagon and hexagon equations:

$$\Phi^{123} \cdot (1\Delta 1)(\Phi) \cdot \Phi^{234} = (\Delta 11)(\Phi) \cdot (11\Delta)(\Phi)$$

$$(\Delta 1)(R^\pm) = \Phi^{123}(R^\pm)^{23}(\Phi^{-1})^{132}(R^\pm)^{13}\Phi^{312}$$

As it turns out, the solution for R is easy and nearly canonical. But finding an associator Φ is rather difficult. There is a closed-form integral expression Φ^{KZ} due to Drinfel’d (1990) but one encounters the same not-too-well-understood multiple ζ numbers. There is a rather complicated iterative procedure for finding an associator (Drinfel’d 1991, Bar-Natan 1998). On a computer it had been used to find an associator up to degree 7. There is also closed-form associator that works only with the Lie superalgebra $\mathfrak{gl}(1|1)$ (Lieberum 2002). But it remains an open

problem to find a closed-form formula for a rational associator (existence by Drienfel'd (1991) and Bar-Natan (1998)).

On the positive side, we should note that the end result, the invariant Z_3 , is independent of the choice of Φ and that $Z_3 = Z_1$.

There is an alternative (more symmetric and intrinsically three dimensional, but less well-documented) description of the theory of associators in terms of knotted trivalent graphs (Bar-Natan and Thurston). There ought to be a perturbative invariant associated with knotted trivalent graphs in the spirit of the last subsection and such an invariant should lead to a simple proof that $Z_2 = Z_3 = Z_1$. But the $\mathcal{E}(D)$ factors remain untamed in this case.

Step-by-Step Integration

The last approach for proving the fundamental theorem is the most natural and historically the first. But here it is last because it is yet to lead to an actual proof. A weight system $W: \mathcal{A}_m^r \rightarrow \mathbb{Q}$ is an invariant of m -singular knots. We want to show that it is the m th derivative of an invariant V of nonsingular knots. It is natural to try to integrate W step by step, first finding an invariant V^{m-1} of $(m-1)$ -singular knots whose derivative in the sense of [1] is W , then an invariant V^{m-2} of $(m-2)$ -singular knots whose derivative is V^{m-1} , and so on all the way up to an invariant $V^0 = V$ whose m th derivative will then be W . If proven, the following conjecture would imply that such an inductive procedure can be made to work:

Conjecture 15 (Hutchings 1998). *If V^r is a once-integrable invariant of r -singular knots, then it is also twice integrable. That is, if there is an invariant V^{r-1} of $(r-1)$ -singular knots whose derivative is V^r , then there is an invariant V^{r-2} of $(r-2)$ -singular knots whose second derivative is V^r .*

Hutchings (1998) reduced this conjecture to a certain appealing topological statement and further to a certain combinatorial-algebraic statement about the vanishing of a certain homology group H^1 which is probably related to Kontsevich's graph homology complex (Kontsevich 1994) (Kontsevich's H^0 is \mathcal{A} , so this is all in the spirit of many deformation theory problems where H^0 enumerates infinitesimal deformations and H^1 is the obstruction to globalization). Hutchings (1998) was also able to prove the vanishing of H^1 (and hence reprove the fundamental theorem) in the simpler case of braids. But no further progress has been made along these lines since then.

Some Further Directions

We would like to touch upon a number of significant further directions in the theory of finite-type invariants and describe each of those only briefly; the reader is referred to the "Further reading" section for more information.

The Original "Vassiliev" Perspective

V A Vassiliev came to the study of finite-type knot invariants by studying the infinite-dimensional space of all immersions of a circle into \mathbb{R}^3 and the topology of the "discriminant," the locus of all singular immersions within the latter space (Vassiliev 1990, 1992). Vassiliev studied the topology of the complement of the discriminant (the space of embeddings) using a certain spectral sequence and found that certain terms in it correspond to finite-type invariants. This later got related to the Goodwillie calculus and back to the configuration spaces discussed in the last section. See Volic (2004).

Interdependent Modifications

The standard definition of finite-type invariants is based on modifying a knot by replacing over (or under) crossings with under (or over) crossings. Goussarov (1998) generalized this by allowing arbitrary modifications done to a knot – just take any segment of the knot and move it anywhere else in space. The resulting new "finite-type" theory turns out to be equivalent to the old one though with a factor of 2 applied to the grading (so an "old" type m invariant is a "new" type $2m$ invariant and vice versa). (see also Bar-Natan (2001) and Conant (2003)).

n -Equivalence, Commutators, and Claspers

While little is known about the overall power of finite-type invariants, much is known about the power of type n -invariants for any given n . Goussarov (1993) defined the notion of n -equivalence: two knots are said to be " n -equivalent" if all their type n -invariants are the same. This equivalence relation is well understood both in terms of commutator subgroups of the pure braid group (Stanford 1998, Ng and Stanford 1999) and in terms of Habiro's calculus of surgery over "claspers" (Habiro 2000) (the latter calculus also gives a topological explanation for the appearance of Jacobi diagrams). In particular, already Goussarov (1993) shows that the set of equivalence classes of knots modulo n -equivalence is a finitely generated abelian group G_n under the operation of connected sum, and the rank of that group is equal to the dimension of the space of type n -invariants.

Ng (1998) has shown that ribbon knots generate an index 2 subgroup of G_n .

Polynomiality and Gauss Sums

Goussarov (1998) (see also Goussarov–Polyak–Viro (2001)) found an intriguing way to compute finite-type invariants from a Gauss diagram presentation of a knot, showing in particular that finite-type invariants grow as polynomials in the number of crossings n and can be computed in polynomial time in n (though actual computer programs are still missing!).

Gauss diagrams are obtained from knot diagrams in much of the same way as Chord diagrams are obtained from singular knots, except all crossings are counted and not just the double points, and certain over/under and sign information is associated with each crossing/chord so that the knot diagram can be recovered from its Gauss diagram. In the example below (Figure 8), we also dashed a subdiagram of the Gauss diagram equivalent to the chord diagram shown in Figure 7.

If G is a Gauss diagram and D is a chord diagram, then let $\langle D, G \rangle$ be the number of subdiagrams of G equivalent to D , counted with appropriate signs (to be precise, we also need to base the diagrams involved and count subdiagrams that respect the basing).

Theorem 16 (Goussarov 1998, Goussarov *et al.* 2000). *If V is a type m invariant, then there are finitely many (based) chord diagrams D_i with at most m chords and rational numbers α_i so that $V(K) = \sum_i \alpha_i \langle D_i, G \rangle$ whenever G is a Gauss diagram representing a knot K .*

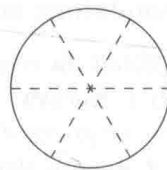


Figure 7 A chord diagram.

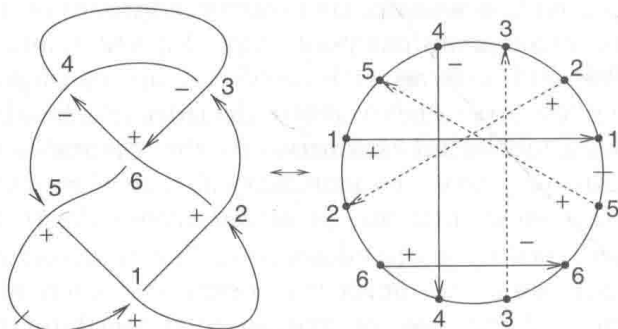


Figure 8 A knot and its Gauss diagram.

Computing the Kontsevich Integral

While the Kontsevich integral Z_1 is a cornerstone of the theory of finite-type invariants, it has been computed for surprisingly few knots. Even for the unknot, the result is nontrivial:

Theorem 17 (“Wheels,” Bar-Natan *et al.* 2000, 2003). *The framed Kontsevich integral of the unknot, $Z_1^F(\bigcirc)$, expressed in terms of diagrams in $\hat{\mathcal{B}}$, is given by $\Omega = \exp_{\sqcup} \sum_{n=1}^{\infty} b_{2n} \omega_{2n}$, where the “modified Bernoulli numbers” b_{2n} are defined by the power series expansion $\sum_{n=0}^{\infty} b_{2n} x^{2n} = (1/2) \log(\sinh x/2)/(x/2)$, the “ $2n$ -wheel” ω_{2n} is the free Jacobi diagram made of a $2n$ -gon with $2n$ legs (so, e.g., $\omega_6 = \bigcirc$), and where \exp_{\sqcup} means “exponential in the disjoint union sense.”*

Closed-form formulas have also been given for the Kontsevich integral of framed unknots, the Hopf link and Hopf chains.

Theorem 17 has a companion that utilizes the same element Ω , the “wheeling” theorem (Bar-Natan *et al.* 2000, 2003). The wheeling theorem “upgrades” the vector space isomorphism $\chi: \mathcal{B} \rightarrow \mathcal{A}$ to an algebra isomorphism and is related to the Duflo isomorphism of the theory of Lie algebras. It is amusing to note that the wheeling theorem (and hence Duflo’s theorem in the metrized case) follows using finite-type techniques from the “ $1 + 1 = 2$ on an abacus” identity (Figure 9).

Taming the Kontsevich Integral

While explicit calculations are rare, there is a nice structure theorem for the values of the Kontsevich integral, saying that for a knot K and up to any fixed number of loops in the Jacobi diagrams, $\chi^{-1} Z_1(K)$ can be described by finitely many rational functions (with denominators powers of the Alexander polynomial) which dictate the placement of the legs. This structure theorem was conjectured in Rozansky (2003), proven in Kricker (2000), and partially generalized to links in Garoufalidis and Kricker (2004).

The Rozansky–Witten Theory

One way to construct linear functionals on \mathcal{A} (and hence finite-type invariants) is using Lie algebras and representations as discussed earlier; much of our insight about \mathcal{A} comes this way. But there is another construction for such functionals (and hence invariants), due to Rozansky and Witten (1997), using contractions of curvature tensors on hyper-Kähler

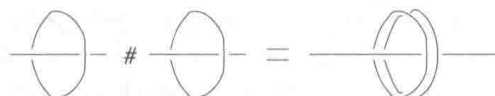


Figure 9 A knot theoretic $1 + 1 = 2$.

manifolds. Very little is known about the Rozansky–Witten approach; in particular, it is not known if it is stronger or weaker than the Lie algebraic approach. For an application of the Rozansky–Witten theory back to hyper-Kähler geometry check Hitchin and Sawon (2001), and for a unification of the Rozansky–Witten approach with the Lie algebraic approach (albeit at a categorical level) check Roberts and Willetton (in preparation).

The Melvin–Morton Conjecture and the Volume Conjecture

The Melvin–Morton conjecture (stated Melvin and Morton (1995), proven Bar-Natan and Garoufalidis (1996)) says that the Alexander polynomial can be read off certain coefficients of the colored Jones polynomial. The Kashaev–Murakami–Murakami volume conjecture (stated Kashaev (1997) and J Murakami and H Murakami (2001), unproven) says that a certain asymptotic growth rate of the colored Jones polynomial is the hyperbolic volume of the knot complement.

Both conjectures are not directly about finite-type invariants but both have ramifications to the theory of finite-type invariants. The Melvin–Morton conjecture was first proven using finite-type invariants and several later proofs and generalizations (see (Bar-Natan)) also involve finite-type invariants. The volume conjecture would imply, in particular, that the hyperbolic volume of a knot complement can be read from that knot’s finite-type invariants, and hence finite-type invariants would be at least as strong as the volume invariant.

A particularly noteworthy result and direction for further research is Gukov’s (preprint) recent unification of these two conjectures under the Chern–Simons umbrella (along with some relations to three-dimensional quantum gravity).

Beyond Knots

For lack of space, we have restricted ourselves here to a discussion of finite-type invariants of knots. But the basic “differentiation” idea of the first section calls for generalization, and indeed it has been generalized extensively. We will only make a few quick comments.

Finite-type invariants of homotopy links (links where each component is allowed to move across itself freely) and of braids are extremely well behaved. They separate, they all come from Lie algebraic constructions and in the case of braids, step-by-step integration as discussed previously works (for homotopy links the issue was not studied).

Finite-type invariants of 3-manifolds and especially of integral and rational homology spheres have been

studied extensively and the picture is nearly a complete parallel of the picture for knots. There are several competing definitions of finite-type invariants, and they all agree up to regrading. There are weight systems and they are linear functionals on a space $\mathcal{A}(\emptyset)$ which is a close cousin of \mathcal{A} and \mathcal{B} and is related to Lie algebras and hyper-Kähler manifolds in a similar way. There is a notion of a “universal” invariant, and there are several constructions; they all agree or are conjectured to agree, and they are related to the Chern–Simons–Witten theory.

Finite-type invariants were studied for several other types of topological objects, including knots within other manifolds, higher-dimensional knots, virtual knots, plane curves and doodles and more (see Bar-Natan).

Acknowledgments

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See also: Finite-Type Invariants of 3-Manifolds; Knot Invariants and Quantum Gravity; Kontsevich Integral; Mathematical Knot Theory; von Neumann Algebras: Introduction, Modular Theory, and Classification Theory.

Further Reading

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Finite-Type Invariants of 3-Manifolds

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Introduction

Physics Background and Motivation

Suppose G is a semisimple compact Lie group and M a closed oriented 3-manifold. Witten (1989) defined quantum invariants by the path integral over all G -connections A :

$$Z(M, G; k) := \int \exp(\sqrt{-1}k \text{CS}(A)) \mathcal{D}A$$

where k is an integer and $\text{CS}(A)$ is the Chern–Simons functional,

$$\text{CS}(A) = \frac{1}{4\pi} \int_M \text{tr} \left(A \wedge dA + \frac{2}{3} A^3 \right)$$

The path integral is not mathematically rigorous. According to the stationary-phase approximation in quantum field theory, in the limit $k \rightarrow \infty$ the path integral decomposes as a sum of contributions from the flat connections:

$$Z(M, G; k) \sim \sum_{\text{flat connections } f} Z^{(f)}(M, G; k) \quad \text{as } k \rightarrow \infty$$

Each contribution is $\exp(2\pi\sqrt{-1}k \text{CS}(f))$ times a power series in $1/k$. The contribution from the trivial connection is important, especially for rational homology 3-spheres, and the coefficients of the powers $(1/k)^n$, calculated using $(n+1)$ -loop Feynman diagrams by quantum field theory techniques, are known as perturbative invariants.

Mathematical Theories

A mathematically rigorous theory of quantum invariants $Z(M, G; k)$ was pioneered by Reshetikhin and Turaev in 1990 (see Turaev (1994)). A number-theoretical expansion of the quantum invariants into power series that should correspond to the perturbative invariants was given by Ohtsuki (in the case of sl_2 , and general simple Lie algebras

by the author) in 1994. This led him to introducing finite-type invariant (FTI) theory for 3-manifolds. A universal perturbative invariant was constructed by Le–Murakami–Ohtsuki (LMO) in 1995; it is universal for both finite-type invariants and quantum invariants, at least for homology 3-spheres. Rozansky in 1996 defined perturbative invariants using Gaussian integral, very close in the spirit to the original physics point of view. Later Habiro (for sl_2 and Habiro and the author for all simple Lie algebras) found a finer expansion of quantum invariants, known as the cyclotomic expansion, but no physics origin is known for the cyclotomic expansion. The cyclotomic expansion helps to show that the LMO invariant dominates all quantum invariants for homology 3-spheres.

The purpose of this article is to give an overview of the mathematical theory of finite-type and perturbative invariants of 3-manifolds.

Conventions and Notations

All vector spaces are assumed to be over the ground field \mathbb{Q} of rational numbers, unless otherwise stated. For a graded space A , let $\text{Gr}_n A$ be the subspace of grading n and $\text{Gr}_{\leq n} A$ the subspace of grading $\leq n$. For $x \in A$, let $\text{Gr}_n x$ and $\text{Gr}_{\leq n} x$ be the projections of x onto, respectively, $\text{Gr}_n A$ and $\text{Gr}_{\leq n} A$.

All 3-manifolds are supposed to be closed and oriented. A 3-manifold M is an integral homology 3-sphere (ZHS) if $H_1(M, \mathbb{Z}) = 0$; it is a rational homology 3-sphere (QHS) if $H_1(M, \mathbb{Q}) = 0$. For a framed link L in a 3-manifold M denote M_L the 3-manifold obtained from M by surgery along L (see e.g., Turaev (1994)).

Finite-Type Invariants

After its introduction by Ohtsuki in 1994, the theory of FTIs of 3-manifolds has been developed rapidly by many authors. Later Goussarov and Habiro independently introduced clasper calculus, or Y -surgery, which provides a powerful geometric technique and deep insight in the theory. Y -surgery, corresponding to the commutator in group theory, naturally gives rise to 3-valent graphs.

Generality on FTIs

Decreasing filtration In a theory of FTIs, one considers a class of objects, and a “good” decreasing filtration $\mathcal{F}_0 \supset \mathcal{F}_1 \supset \mathcal{F}_2 \supset \cdots$ on the vector space $\mathcal{F} = \mathcal{F}_0$ spanned by these objects. An invariant of the objects with values in a vector space is of order less than or equal to n if its restriction to \mathcal{F}_{n+1} is 0; it is of finite type if it is of order $\leq n$ for some n . An invariant has order n if it is of order $\leq n$ but not $\leq n-1$. Good here means at least the space of FTI of each order is finite dimensional. It is desirable to have an algorithm of polynomial time to calculate every FTI. In addition, one wants the set of FTIs to separate the objects (completeness).

The space of invariants of order $\leq n$ can be identified with the dual space of $\mathcal{F}_0/\mathcal{F}_{n+1}$; its subspace $\mathcal{F}_n/\mathcal{F}_{n+1}$ is isomorphic to the space of invariants of order $\leq n$ modulo the space of invariants of order $\leq n-1$. Informally, one can say that $\mathcal{F}_n/\mathcal{F}_{n+1}$ is more or less the set of invariants of order n .

Elementary moves, the knot case Usually the filtrations are defined using “independent elementary moves.” For the class of knots the elementary move is given by crossing change. Any two knots can be connected by a finite sequence of such moves. The idea is if $K, K' \in \mathcal{F}_n$, the n th term of the filtration, then $K - K' \in \mathcal{F}_{n+1}$, where K' is obtained from K by an elementary move. Formal definition is as follows. Suppose S is a set of double points of a knot diagram D . Let

$$[D, S] = \sum_{S' \subset S} (-1)^{\#S'} D_{S'}$$

where the sum is over all subsets S' of S , including the empty set, $D_{S'}$ is the knot obtained by changing the crossing at every point in S' , and $\#S'$ is the number of elements of S' . Then \mathcal{F}_n is the vector space spanned by all elements of the form $[D, S]$ with $\#S = n$. For the knot case, the Kontsevich integral is an invariant that is universal for all FTIs (see Bar-Natan (1995)).

Ohtsuki's Definition of FTIs for ZHS

An elementary move here is a surgery along a knot: $M \rightarrow M_K$, where K is a framed knot in a ZHS M . A collection of moves corresponds to surgery on a framed link. To always remain in the class of ZHS we need to restrict ourselves to unit-framed and algebraically split links, that is, framed links in ZHS each component of which has framing ± 1 and the linking number of every two components is 0. It is easy to prove that a link L

in a ZHS M is unit-framed and algebraically split if and only if $M_{L'}$ is a ZHS for every sublink L' of L . For a unit-framed, algebraically split link L in a ZHS M define

$$[M, L] = \sum_{L' \subset L} (-1)^{\#L'} M_{L'}$$

which is an element in the vector space \mathcal{M} freely spanned by ZHS.

For a non-negative integer n let $\mathcal{F}_n^{\text{AS}}$ be the subspace of \mathcal{M} spanned by $[M, L]$ with $\#L = n$. Then the descending filtration $\mathcal{M} = \mathcal{F}_0^{\text{AS}} \supset \mathcal{F}_1^{\text{AS}} \supset \mathcal{F}_2^{\text{AS}} \supset \cdots$ defines a theory of FTIs on the class of ZHS.

Theorem 1

- (i) (Ohtsuki) *The dimension of $\mathcal{F}_n(\mathcal{M})$ is finite for every n .*
- (ii) (Garoufalidis–Ohtsuki) *One has $\mathcal{F}_{3n+1}(\mathcal{M}) = \mathcal{F}_{3n+2}(\mathcal{M}) = \mathcal{F}_{3n+3}(\mathcal{M})$.*

The orders of FTIs in this theory are multiples of 3. The first nontrivial invariant, which is the only (up to scalar) invariant of degree 3, is the Casson invariant.

The Goussarov–Habiro Definition

Y-surgery or clasper surgery Consider the standard Y-graph Y and a small neighborhood $N(Y)$ of it in the standard \mathbb{R}^2 (see Figure 1). Denote by $L(Y)$ the six-component framed link diagram in $N(Y) \subset \mathbb{R}^3$, each component of which has framing 0 in \mathbb{R}^3 (see Figure 1).

A framed Y-graph C in a 3-manifold M is the image of an embedding of $N(Y)$ into M . The surgery of M along the image of the six-component link $L(Y)$ is called a Y-surgery along C , denoted by M_C . If one of the leaves bounds a disk in M whose interior is disjoint from the graph, then M_C is homeomorphic to M .

Matveev in 1987 proved that two 3-manifolds M and M' are related by a finite sequence of Y-surgeries if and only if there is an isomorphism from $H_1(M, \mathbb{Z})$ onto $H_1(M', \mathbb{Z})$ preserving the

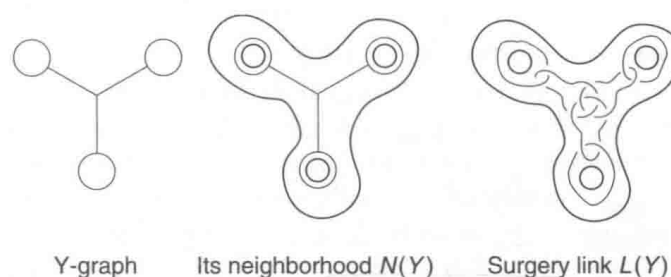


Figure 1 Y-graph.

linking form on the torsion group. It is natural to partition the class of 3-manifolds into subclasses of the same H_1 and the same linking form.

Goussarov–Habiro filtrations For a 3-manifold M denote by $\mathcal{M}(M)$ the vector space spanned by all 3-manifolds with H_1 and linking form the same as those of M . Define, for a set S of Y-graphs in M , $[M, S] = \sum_{S' \subset S} (-1)^{\#S'} M_{S'}$, and $\mathcal{F}_n^Y \mathcal{M}(M)$ the vector space spanned by all $[N, S]$ such that N is in $\mathcal{M}(M)$ and $\#S = n$. The following theorem of Goussarov and Habiro (Goussarov 1999, Garoufalidis *et al.* 2001, Habiro 2000) shows that the FTI theory based on Y-surgery is the same as the one of Ohtsuki in the case of ZHS.

Theorem 2 *For the case $\mathcal{M} = \mathcal{M}(S^3)$, one has $\mathcal{F}_{2n-1}^Y = \mathcal{F}_{2n}^Y = \mathcal{F}_{3n}^{AS}$.*

The Fundamental Theorem of FTIs of ZHS

Jacobi diagrams A closed Jacobi diagram is a vertex-oriented trivalent graph, that is, a graph for which the degree of each vertex is equal to 3 and a cyclic order of the three half-edges at every vertex is fixed. Here, multiple edges and self-loops are allowed. In pictures, the orientation at a vertex is the clockwise orientation, unless otherwise stated. The “degree” of Jacobi diagram is half the number of its vertices.

Let $\text{Gr}_n \mathcal{A}(\emptyset)$, $n \geq 0$, be the vector space spanned by all closed Jacobi diagrams of degree n , modulo the antisymmetry (AS) and Jacobi (IHJ) relations (see Figure 2).

The universal weight map W Suppose D is a closed Jacobi diagram of degree n . Embedding D into $\mathbb{R}^3 \subset S^3$ arbitrarily and then projecting down onto \mathbb{R}^2 in general position, one can describe D by a diagram, with over/under-crossing information at every double point just as in the case of a link diagram. We can assume that the orientation at every vertex of D is given by a clockwise cyclic order. From the image of D , construct a set G of $2n$ Y-graphs as in

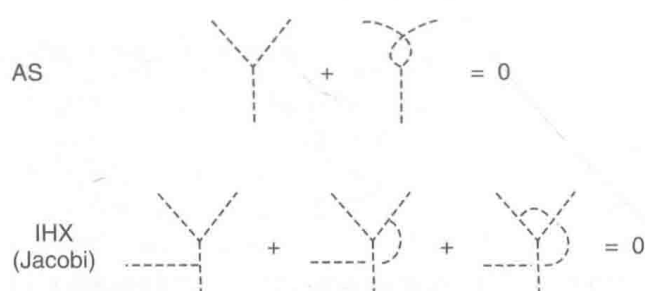


Figure 2 The AS and IHJ relations.

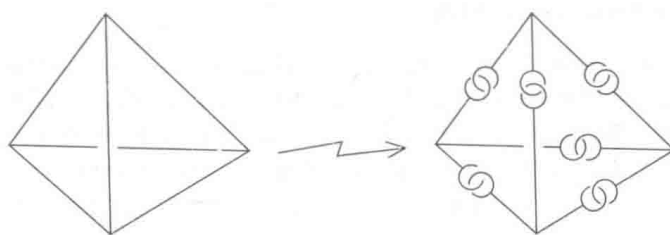


Figure 3 The weight map.

Figure 3. Here only the cores of a Y-graph are drawn, with the convention that each framed Y-graph is a small neighborhood of its core in \mathbb{R}^2 .

If G' is a proper subset of G , then in G' there is a Y-graph, one of the leaves of which bounds a disk, hence $S_{G'}^3 = S^3$. Thus, $W(D) := [S^3, G] = S_G^3 - S^3$. By definition, $W(D) \in \mathcal{F}_{2n}^Y$; it might depend on the embedding of D into \mathbb{R}^3 , but one can show that $W(D)$ is well defined in $\mathcal{F}_{2n}^Y / \mathcal{F}_{2n+1}^Y$. The map W was first constructed by Garoufalidis and Ohtsuki in the framework of \mathcal{F}^{AS} .

Fundamental theorem

Theorem 3 (Lê *et al.* 1998, Lê 1997). *The map W descends to a well-defined linear map $W: \text{Gr}_n \mathcal{A}(\emptyset) \rightarrow \mathcal{F}_{2n}^Y / \mathcal{F}_{2n+1}^Y$ and moreover, is an isomorphism between the vector spaces $\text{Gr}_n \mathcal{A}(\emptyset)$ and $\mathcal{F}_{2n}^Y / \mathcal{F}_{2n+1}^Y$, for $\mathcal{M} = \mathcal{M}(S^3)$.*

The theorem essentially says that the set of invariants of degree $2n$ is dual to the space of closed Jacobi diagram $\text{Gr}_n \mathcal{A}(\emptyset)$. The proof is based on the LMO invariant (see the next section).

A \mathbb{Q} -valued invariant I of order $\leq 2n$ restricts to a linear map from $\mathcal{F}_{2n} / \mathcal{F}_{2n+1}$ to \mathbb{Q} . The composition of I and W is a functional on $\text{Gr}_n \mathcal{A}(\emptyset)$ called the “weight system” of I . The theorem shows that every linear functional on $\text{Gr}_{\leq n} \mathcal{A}(\emptyset)$ is the weight of an invariant of order $\leq 2n$.

Relation to knot invariants Under the map that sends an (unframed) knot $K \subset S^3$ to the ZHS obtained by surgery along K with framing 1, an invariant of degree $\leq 2n$ (in the \mathcal{F}^Y theory) of ZHS pulls back to an invariant of order $\leq 2n$ of knots. This was conjectured by Garoufalidis and proved by Habegger.

Other classes of rational homology 3-spheres Actually, the theorem was first proved in the framework of \mathcal{F}^{AS} . Clasper surgery theory allows Habiro (2000) to generalize the fundamental theorem to QHS: for M a QHS, the universal weight map $W: \text{Gr}_n \mathcal{A}(\emptyset) \rightarrow \mathcal{F}_{2n} \mathcal{M}(M) / \mathcal{F}_{2n+1} \mathcal{M}(M)$, defined similarly as

in the case of $\mathbb{Z}HS$, is an isomorphism, and $\mathcal{F}_{2n-1}\mathcal{M}(M) = \mathcal{F}_{2n}\mathcal{M}(M)$.

Other filtrations and approaches Other equivalent filtrations were introduced (and compared) by Garoufalidis, Garoufalidis and Levine (1997), and Garoufalidis–Goussarov–Polyak (2001). Of importance is the one using subgroups of mapping class groups in Garoufalidis and Levine (1997). A theory of n -equivalence was constructed by Goussarov and Habiro that encompasses many geometric aspects of FTIs of 3-manifolds (Habiro 2000, Goussarov 1999). Cochran and Melvin (2000) extended the original Ohtsuki definition to manifolds with homology, using algebraically split links, but the filtrations are different from those of Goussarov–Habiro.

The Le–Murakami–Ohtsuki Invariant

Jacobi Diagrams

An open Jacobi diagram is a vertex-oriented univalent graph, that is, a graph with univalent and trivalent vertices together with a cyclic ordering of the edges incident to the trivalent vertices. A univalent vertex is also called “a leg.” The degree of an open Jacobi diagram is half the number of vertices (trivalent and univalent). A Jacobi diagram based on X , a compact oriented 1-manifold, is a graph D together with a decomposition $D = X \cup \Gamma$, such that D is the result of gluing all the legs of an open Jacobi diagram Γ to distinct interior points of X . The degree of D , by definition, is the degree of Γ . In Figure 4 X is depicted by bold lines. Let $\mathcal{A}^f(X)$ be the space of Jacobi diagrams based on X modulo the usual antisymmetry, Jacobi and the new STU relations. The completion of $\mathcal{A}^f(X)$ with respect to degree is denoted by $\mathcal{A}(X)$.

When X is a set of m -ordered oriented intervals, denote $\mathcal{A}(X)$ by \mathcal{P}_m , which has a natural algebra structure where the product DD' of two Jacobi diagrams is defined by stacking D on top of D' (concatenating the corresponding oriented intervals). When X is a set of m -ordered oriented circles, denote $\mathcal{A}(X)$ by \mathcal{A}_m . By identifying the two endpoints of each interval, one gets a map $pr: \mathcal{P}_m \rightarrow \mathcal{A}_m$, which is an isomorphism if $m = 1$ (see Bar-Natan (1995)).



Figure 4 The STU relation.

For $x \in \mathcal{A}_m$ and $y \in \mathcal{A}_1$, the connected sum is defined by $x \#_m y := pr((pr^{-1}x)(pr^{-1}y)^{\otimes m})$, where $(pr^{-1}y)^{\otimes m}$ is the element in \mathcal{P}_m with $pr^{-1}y$ on each oriented interval.

Symmetrization maps Let \mathcal{B}_m be the vector space spanned by open Jacobi diagrams whose legs are labeled by elements of $\{1, 2, \dots, m\}$, modulo the antisymmetry and Jacobi relations. One can define an analog of the Poincaré–Birkhoff–Witt isomorphism $\chi: \mathcal{B}_m \rightarrow \mathcal{P}_m$ as follows. For a diagram D , $\chi(D)$ is obtained by taking the average over all possible ways of ordering the legs labeled by j and attaching them to the j th oriented interval. It is known that χ is a vector space isomorphism (Bar-Natan (1995)).

The Framed Kontsevich Integral of Links

For an m -component framed link $L \subset \mathbb{R}^3$, the (framed version of the) Kontsevich integral $Z(L)$ is an invariant taking values in \mathcal{A}_m (see, e.g., Ohtsuki (2002)). Let $\nu := Z(K)$, when K is the unknot with framing 0, and $\tilde{Z}(L) := Z(L) \#_m \nu$. An explicit formula for ν is given in Bar-Natan *et al.* (2003).

Removing Solid Loops: The Maps ι_n

Suppose $x \in \mathcal{B}_m$ is an open Jacobi diagram with legs labeled by $\{1, \dots, m\}$. If the number of vertices of any label is different from $2n$, or if the degree of $D > (m+1)n$, we set $\iota_n(D) = 0$. Otherwise, partitioning the $2n$ vertices of each label into n pairs and identifying points in each pair, from x we get a trivalent graph which may contain some isolated loops (no vertices) and which depends on the partition. Replacing each isolated loop by a factor $-2n$, and summing up over all partitions, we get $\iota_n(D) \in \text{Gr}_{\leq n} \mathcal{A}(\emptyset)$.

For $x \in \mathcal{A}_m$, choose $y \in \mathcal{P}_m$ such that $pr(y) = x$. Using the isomorphism χ we pull back $\chi^{-1}y \in \mathcal{B}_m$. Define $\iota_n(x) := \iota_n(\chi^{-1}y)$. One can prove that $\iota_n(x)$ does not depend on the choice of the preimage y of x . Note that ι_n lowers the degree by nm .

Definition of the Le–Murakami–Ohtsuki Invariant Z^{LMO}

In $\mathcal{A}(\emptyset) := \prod_{n=0}^{\infty} \text{Gr}_n \mathcal{A}(\emptyset)$ let the product of two Jacobi diagrams be their disjoint union. In addition, define the coproduct $\Delta(D) = 1 \otimes D + D \otimes 1$ for D a connected Jacobi diagram. Then $\mathcal{A}(\emptyset)$ is a commutative cocommutative graded Hopf algebra.

For the unknot U_{\pm} with framing ± 1 , one has $\iota_n(\tilde{Z}(U_{\pm})) = (\mp 1)^n + (\text{terms of degree } \geq 1)$; hence, their inverses exist. Suppose the linking matrix of an

oriented framed link $L \subset \mathbb{R}^3$ has σ_+ positive eigenvalues and σ_- negative eigenvalues. Define

$$\Omega_n(L) = \frac{\iota_n(\check{Z}(L))}{(\iota_n(\check{Z}(U_+)))^{\sigma_+} (\iota_n(\check{Z}(U_-)))^{\sigma_-}} \in \text{Grad}_{\leq n}(\mathcal{A}(\emptyset)) \quad [1]$$

Theorem 4 (Lê *et al.* 1998). $\Omega_n(L)$ is an invariant of the 3-manifold $M = S_L^3$.

We can combine all the Ω_n to get a better invariant:

$$Z^{\text{LMO}}(M) := 1 + \text{Grad}_1(\Omega_1(M)) + \cdots + \text{Grad}_n(\Omega_n(M)) + \cdots \in \mathcal{A}(\emptyset)$$

For M a QHS, we also define

$$\hat{Z}^{\text{LMO}}(M) := 1 + \frac{\text{Grad}_1(\Omega_1(M))}{d(M)} + \cdots + \frac{\text{Grad}_n(\Omega_n(M))}{d(M)^n} + \cdots$$

where $d(M)$ is the cardinality of $H_1(M, \mathbb{Z})$.

Proposition 1 (Lê *et al.* 1998). Both $Z^{\text{LMO}}(M)$ and $\hat{Z}^{\text{LMO}}(M)$ (when defined) are group-like elements, that is,

$$\Delta(Z^{\text{LMO}}(M)) = Z^{\text{LMO}}(M) \otimes Z^{\text{LMO}}(M)$$

$$\Delta(\hat{Z}^{\text{LMO}}(M)) = \hat{Z}^{\text{LMO}}(M) \otimes \hat{Z}^{\text{LMO}}(M)$$

Moreover, $\hat{Z}^{\text{LMO}}(M_1 \# M_2) = \hat{Z}^{\text{LMO}}(M_1) \times \hat{Z}^{\text{LMO}}(M_2)$.

Universality Properties of the LMO Invariant

Let us restrict ourselves to the case of ZHS.

Theorem 5 (Lê 1997). The less than or equal to n degree part $\text{Gr}_{\leq n} Z^{\text{LMO}}$ is an invariant of degree $2n$. Any invariant of degree $\leq 2n$ is a composition $w(\text{Gr}_{\leq n} Z^{\text{LMO}})$, where $w: \text{Gr}_{\leq n} \mathcal{A}(\emptyset) \rightarrow \mathbb{Q}$ is a linear map.

Clasper calculus (or Y -surgery) theory allows Habiro to extend the theorem to rational homology 3-spheres.

The Aarhus Integral

The Aarhus integral (ca. 1998) of Bar-Natan, Garoufalidis, Rozansky and Thurston, based on a theory of formal integration, calculates the LMO invariant of rational homology 3-spheres. The formal integration theory has a conceptual flavor and helps to relate the LMO invariant to perturbative expansions of quantum invariants. We give here the definition for the case when one does surgery on

a knot K with nonzero framing b . The link case is similar (see Bar-Natan *et al.* (2002a, b)).

When K is a knot, $\check{Z}(K)$ is an element of $\mathcal{A}_1 \equiv \mathcal{P}_1 \equiv \mathcal{B}_1$. Note that \mathcal{B}_1 is an algebra where the product is the disjoint union \sqcup . Since the framing is b , one has

$$\check{Z}(K) = \exp_{\sqcup}(b w_1/2) \sqcup Y$$

where w_1 is the “dashed interval” (the only connected open Jacobi diagram without trivalent vertex), and Y is an element in \mathcal{B} every term of which must have at least one trivalent vertex. For uni-trivalent graphs $C, D \in \mathcal{B}_1$ let

$$\langle C, D \rangle = \begin{cases} 0 & \text{if the numbers of legs of } C, D \\ & \text{are different} \\ \text{sum of all ways to glue legs of } C \text{ and } D & \text{together} \end{cases}$$

One defines $\int^{\text{FG}} \check{Z}(K) := \langle \exp_{\sqcup}(-w_1/2b), Y \rangle$. Then

$$\int^{\text{FG}} \check{Z}(K) = \sum_{n=0}^{\infty} \frac{\text{Gr}_n(\iota_n \check{Z}(K))}{(-b)^n}$$

Hence,

$$\hat{Z}^{\text{LMO}}(S_K^3) = \frac{\int^{\text{FG}} \check{Z}(K)}{\int^{\text{FG}} \check{Z}(U_{\text{sign}(b)})}$$

Other Approaches

Another construction of a universal perturbative invariant based on integrations over configuration spaces, closer to the original physics approach but harder to calculate because of the lack of a surgery formula, was developed by Axelrod and Singer, Kontsevich, Bott and Cattaneo, Kuperberg and Thurston (see Axelrod and Singer (1992), Bott and Cattaneo (1998)).

Quantum Invariants and Perturbative Expansion

Fix a simple (complex) Lie algebra \mathfrak{g} of finite dimension. Using the quantized enveloping algebra of \mathfrak{g} one can define quantum link and 3-manifold invariants. We recall here the definition, adapted for the case of roots lattice (projective group case).

Here our q is equal to q^2 in the text book (Jantzen 1995). Fix a root system of \mathfrak{g} . Let X, X_+, Y denote respectively the weight lattice, the set of dominant weights, and the root lattice. We normalize the invariant scalar product in the real vector space of the weight lattice so that the length of any short root is $\sqrt{2}$.

Quantum Link Invariants

Suppose L is a framed oriented link with m -ordered components, then the quantum invariant $J_L(\lambda_1, \dots, \lambda_m)$ is a Laurent polynomial in $q^{1/2D}$, where $\lambda_1, \dots, \lambda_m$ are dominant weights, standing for the simple \mathfrak{g} -modules of highest weights $\lambda_1, \dots, \lambda_m$, and D is the determinant of the Cartan matrix of \mathfrak{g} (see, e.g., Turaev (1994) and Lê (1996)). The Jones polynomial is the case when $\mathfrak{g} = \mathfrak{sl}_2$ and all the λ_i 's are the highest weights of the fundamental representation. For the unknot U with zero framing, one has (here ρ is the half-sum of all positive roots)

$$J_U(\lambda) = \prod_{\text{positive roots } \alpha} \frac{q^{(\lambda+\rho|\alpha)/2} - q^{-(\lambda+\rho|\alpha)/2}}{q^{(\rho|\alpha)/2} - q^{-(\rho|\alpha)/2}}$$

We will also use another normalization of the quantum invariant:

$$Q_L(\lambda_1, \dots, \lambda_m) := J_L(\lambda_1, \dots, \lambda_m) \times \prod_{j=1}^m J_U(\lambda_j)$$

This definition is good only for $\lambda_j \in X_+$. Note that each $\lambda \in X$ is either fixed by an element of the Weyl group under the dot action (see Humphreys (1978)) or can be moved to X_+ by the dot action. We define $Q_L(\lambda_1, \dots, \lambda_m)$ for arbitrary $\lambda_j \in X$ by requiring that $Q_L(\lambda_1, \dots, \lambda_m) = 0$ if one of the λ_j 's is fixed by an element of the Weyl group, and that $Q_L(\lambda_1, \dots, \lambda_m)$ is component-wise invariant under the dot action of the Weyl group, that is, for every w_1, \dots, w_m in the Weyl group,

$$Q_L(w_1 \cdot \lambda_1, \dots, w_m \cdot \lambda_m) = Q_L(\lambda_1, \dots, \lambda_m)$$

Proposition 2 (Lê 1996). *Suppose $\lambda_1, \dots, \lambda_m$ are in the root lattice Y .*

- (i) (Integrality) *Then $Q_L(\lambda_1, \dots, \lambda_m) \in \mathbb{Z}[q^{\pm 1}]$, (no fractional power).*
- (ii) (Periodicity) *When q is an r th root of 1, then $Q_L(\lambda_1, \dots, \lambda_m)$ is invariant under the action of the lattice group rY , that is, for $y_1, \dots, y_m \in Y$, $Q_L(\lambda_1, \dots, \lambda_m) = Q_L(\lambda_1 + ry_1, \dots, \lambda_m + ry_m)$.*

Quantum 3-Manifold Invariants

Although the infinite sum $\sum_{\lambda_j \in Y} Q_L(\lambda_1, \dots, \lambda_m)$ does not have a meaning, heuristic ideas show that it is invariant under the second Kirby move, and hence almost defines a 3-manifold invariant. The problem is to regularize the infinite sum. One solution is based on the fact that at r th roots of unity, $Q_L(\lambda_1, \dots, \lambda_m)$ is periodic, so we should use

the sum with λ_j 's run over a fundamental set P_r of the action of rY , where

$$P_r := \{x = c_1\alpha_1 + \dots + c_\ell\alpha_\ell \mid 0 \leq c_1, \dots, c_\ell < r\}$$

Here $\alpha_1, \dots, \alpha_\ell$ are basis roots. For a root ξ of unity of order r , let

$$F_L(\xi) = \sum_{\lambda_j \in (P_r \cap Y)} Q_L(\lambda_1, \dots, \lambda_m)|_{q=\xi}$$

If $F_{U_\pm}(\xi) \neq 0$, define

$$\tau_L(\xi) := \frac{F_L(\xi)}{(F_{U_+}(\xi))^{\sigma_+} (F_{U_-}(\xi))^{\sigma_-}}$$

Recall that D is the determinant of the Cartan matrix. Let d be the maximum of the absolute values of entries of the Cartan matrix outside the diagonal.

Theorem 6 (Lê 2003)

- (i) *If the order r of ξ is coprime with dD , then $F_{U_\pm}(\xi) \neq 0$.*
- (ii) *If $F_{U_\pm}(\xi) \neq 0$ then $\tau_M^{P_\mathfrak{g}}(\xi) := \tau_L(\xi)$ is an invariant of the 3-manifold $M = S_L^3$.*

Remark 1 The version presented here corresponds to projective groups. It was defined by Kirby and Melvin for \mathfrak{sl}_2 , Kohno and Takata for \mathfrak{sl}_n , and by Lê (2003) for arbitrary simple Lie algebra. When r is coprime with dD , there is also an associated modular category that generates a topological quantum field theory. In most texts in literature, say Kirillov (1996) and Turaev (1994), another version $\tau^\mathfrak{g}$ was defined. The reason we choose $\tau^{P_\mathfrak{g}}$ is: it has nice integrality and eventually perturbative expansion. For relations between the version $\tau^{P_\mathfrak{g}}$ and the usual $\tau^\mathfrak{g}$, see Lê (2003).

Examples When M is the Poincaré sphere and $\mathfrak{g} = \mathfrak{sl}_2$,

$$\tau_M^{P_{\mathfrak{sl}_2}}(q) = \frac{1}{1-q} \sum_{n=0}^{\infty} q^n (1 - q^{n+1}) \times (1 - q^{n+2}) \dots (1 - q^{2n+1})$$

Here q is a root of unity, and the sum is easily seen to be finite.

Integrality The following theorem was proved for $\mathfrak{g} = \mathfrak{sl}_2$ by Murakami (1995) and for $\mathfrak{g} = \mathfrak{sl}_n$ by Takata–Yokota and Masbaum–Wenzl (using ideas of J Roberts) and for arbitrary simple Lie algebras by Lê (2003).

Theorem 7 *Suppose the order r of ξ is a prime big enough, then $\tau_M^{P_\mathfrak{g}}(\xi)$ is in $\mathbb{Z}[\xi] = \mathbb{Z}[\exp(2\pi i/r)]$.*

Perturbative Expansion

Unlike the link case, quantum 3-manifold invariants can be defined only at certain roots of unity. In general, there is no analytic extension of the function τ_M^{Pg} around $q=1$. In perturbative theory, we want to expand the function τ_M^g around $q=1$ into power series. For QHS, Ohtsuki (for $g=sl_2$) and then the present author (for all other simple Lie algebras) showed that there is a number-theoretical expansion of τ_M^{Pg} around $q=1$ in the following sense.

Suppose r is a big enough prime, and $\xi = \exp(2\pi i/r)$. By the integrality (Theorem 7),

$$\tau_M^{Pg}(\xi) \in \mathbb{Z}[\xi] = \mathbb{Z}[q]/(1+q+q^2+\cdots+q^{r-1})$$

Choose a representative $f(q) \in \mathbb{Z}[q]$ of $\tau_M^{Pg}(\xi)$. Formally substitute $q = (q-1) + 1$ in $f(q)$:

$$f(q) = c_{r,0} + c_{r,1}(q-1) + \cdots + c_{r,n-2}(q-1)^{n-2}$$

The integers $c_{r,n}$ depend on r and the representative $f(q)$. It is easy to see that $c_{r,n} \pmod{r}$ does not depend on the representative $f(q)$ and hence is an invariant of QHS. The dependence on r is a big drawback. The theorem below says that there is a rational number c_n , not depending on r , such that $c_{r,n} \pmod{r}$ is the reduction of either c_n or $-c_n$ modulo r , for sufficiently large prime r . It is easy to see that if such c_n exists, it must be unique. Let s be the number of positive roots of g . Recall that ℓ is the rank of g .

Theorem 8 *For every QHS M , there is a sequence of numbers*

$$c_n \in \mathbb{Z} \left[\frac{1}{(2n+2s)! |H_1(M, \mathbb{Z})|} \right]$$

such that for sufficiently large prime r

$$c_{r,n} \equiv \left(\frac{|H_1(M, \mathbb{Z})|}{r} \right)^\ell c_n \pmod{r}$$

where

$$\left(\frac{|H_1(M, \mathbb{Z})|}{r} \right) = \pm 1$$

is the Legendre symbol. Moreover, c_n is an invariant of order $\leq 2n$.

The series $t_M^{Pg}(q-1) := \sum_{n=0}^{\infty} c_n(q-1)^n$, called the Ohtsuki series, can be considered as the perturbative expansion of the function τ_M^{Pg} at $q=1$. For actual calculation of $t_M^{Pg}(q-1)$, see Lê (2003), Ohtsuki (2002), and Rozansky (1997).

Recovery from the LMO invariant It is known that for any metrized Lie algebra g , there is a linear map $W_g: Gr_n \mathcal{A}(\emptyset) \rightarrow \mathbb{Q}$ (see Bar-Natan (1995)).

Theorem 9 *One has*

$$\sum_{n=0}^{\infty} W_g(Gr_n Z^{LMO}) b^n = t_M^{Pg}(q-1)|_{q=e^b}$$

This shows that the Ohtsuki series $t_M^{Pg}(q-1)$ can be recovered from, and hence totally determined by, the LMO invariant. The theorem was proved by Ohtsuki for sl_2 . For other simple Lie algebras, the theorem follows from the Aarhus integral (see Bar-Natan *et al.* (2002a, b) and Ohtsuki (2002)).

Rozansky's Gaussian Integral

Rozansky (1997) gave a definition of the Ohtsuki series using formal Gaussian integral in the important work. The work is only for sl_2 , but can be generalized to other Lie algebras; it is closer to the original physics ideas of perturbative invariants.

Cyclotomic Expansion

The Habiro Ring

Let us define the Habiro ring $\widehat{\mathbb{Z}[q]}$ by

$$\widehat{\mathbb{Z}[q]} := \lim_{\leftarrow n} \mathbb{Z}[q]/((1-q)(1-q^2)\cdots(1-q^n))$$

Habiro (2002) called it the cyclotomic completion of $\mathbb{Z}[q]$. Formally, $\widehat{\mathbb{Z}[q]}$ is the set of all series of the form

$$f(q) = \sum_{n=0}^{\infty} f_n(q)(1-q)(1-q^2)\cdots(1-q^n)$$

$$f_n(q) \in \mathbb{Z}[q]$$

Suppose U is the set of roots of 1. If $\xi \in U$ then $(1-\xi)(1-\xi^2)\cdots(1-\xi^n)=0$ if n is big enough; hence, one can define $f(\xi)$ for $f \in \widehat{\mathbb{Z}[q]}$. One can consider every $f \in \widehat{\mathbb{Z}[q]}$ as a function with domain U . Note that $f(\xi) \in \mathbb{Z}[\xi]$ is always an algebraic integer. It turns out that $\widehat{\mathbb{Z}[q]}$ has remarkable properties, and plays an important role in quantum topology.

Note that the formal derivative of $(1-q)(1-q^2)\cdots(1-q^n)$ is divisible by $(1-q)(1-q^2)\cdots(1-q^k)$ with $k > (n-1)/2$. This means every element $f \in \widehat{\mathbb{Z}[q]}$ has a derivative $f' \in \widehat{\mathbb{Z}[q]}$, and hence derivatives of all orders in $\widehat{\mathbb{Z}[q]}$. One can then associate to $f \in \widehat{\mathbb{Z}[q]}$ its Taylor series at a root ξ of 1:

$$T_\xi(f) := \sum_{n=0}^{\infty} \frac{f^{(n)}(\xi)}{n!} (q-\xi)^n$$

which can also be obtained by noticing that $(1-q)(1-q^2)\cdots(1-q^n)$ is divisible by $(q-\xi)^k$ if n is bigger than k times the order of ξ . Thus, one has a map $T_\xi: \widehat{\mathbb{Z}[q]} \rightarrow \mathbb{Z}[\xi][[q-\xi]]$.

Theorem 10 (Habiro 2004)

- (i) For each root of unity ξ , the map T_ξ is injective, that is, a function in $\widehat{\mathbb{Z}[q]}$ is determined by its Taylor expansion at a point in the domain U .
- (ii) if $f(\xi) = g(\xi)$ at infinitely many roots ξ of prime power orders, then $f = g$ in $\widehat{\mathbb{Z}[q]}$.

One important consequence is that $\widehat{\mathbb{Z}[q]}$ is an integral domain, since we have the embedding $T_1: \mathbb{Z}[q] \hookrightarrow \mathbb{Z}[[q-1]]$.

In general the Taylor series $T_1 f$ has 0 convergence radius. However, one can speak about p -adic convergence to $f(\xi)$ in the following sense. Suppose the order r of ξ is a power of prime, $r = p^k$. Then it is known that $(\xi - 1)^n$ is divisible by p^m if $n > mk$. Hence, $T_1 f(\xi)$ converges in the p -adic topology, and it can be easily shown that the limit is exactly $f(\xi)$.

The above properties suggest considering $\widehat{\mathbb{Z}[q]}$ as a class of “analytic functions” with domain U .

Quantum Invariants as an Element of $\widehat{\mathbb{Z}[q]}$

It was proved, by Habiro for \mathfrak{sl}_2 and by Habiro with the present author for general simple Lie algebras, that quantum invariants of ZHSs belong to $\widehat{\mathbb{Z}[q]}$ and thus have remarkable integrality properties:

Theorem 11

- (i) For every ZHS M , there is an invariant $I_M^q \in \widehat{\mathbb{Z}[q]}$ such that if ξ is a root of unity for which the quantum invariant $\tau_M^{Pq}(\xi)$ can be defined, then $I_M^q(\xi) = \tau_M^{Pq}(\xi)$.
- (ii) The Ohtsuki series is equal to the Taylor series of I_M^q at 1.

Corollary 1 Suppose M is a ZHS.

- (i) For every root of unity ξ , the quantum invariant at ξ is an algebraic integer, $\tau_M^q(\xi) \in \mathbb{Z}[\xi]$. (No restriction on the order of ξ is required.)
- (ii) The Ohtsuki series $t_M^{Pq}(q-1)$ has integer coefficients. If ξ is a root of order $r = p^k$, where p is prime, then the Ohtsuki series at ξ converges p -adically to the quantum invariant at ξ .
- (iii) The quantum invariant τ_M^{Pq} is determined by values at infinitely many roots of prime power orders and also determined by its Ohtsuki series.
- (iv) The LMO invariant totally determines the quantum invariants τ_M^{Pq} .

Part (ii) was conjectured by R Lawrence for \mathfrak{sl}_2 and first proved by Rozansky (also for \mathfrak{sl}_2). Part (iv) follows from the fact that the LMO invariant determines the Ohtsuki series; it exhibits another universality property of the LMO invariant.

See also: Finite-Type Invariants; Knot Invariants and Quantum Gravity; Lie Groups: General Theory; Quantum 3-Manifold Invariants.

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Floer Homology

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Introduction

Morse theory allows one to reconstruct the homology of a compact manifold B from data obtained from the gradient flow of a function $f: B \rightarrow \mathbb{R}$, the Morse function. The term “Floer homology” is used to describe homology groups that arise from carrying out the same construction, but in a setting where the space B is replaced by an infinite-dimensional manifold (a space of maps, or a space of configurations for a gauge theory), and where the gradient trajectories of the Morse function correspond to solutions of an elliptic differential equation. There are two important types of such homology theories that have been extensively developed, and the study of both was initiated in the 1980s by Andreas Floer. In the first type, the elliptic equation that arises is a Cauchy–Riemann equation, whose solutions are pseudoholomorphic maps from a two-dimensional domain into a symplectic manifold. In the second type, the elliptic equation is an equation of gauge theory on a 4-manifold: either the anti-self-dual Yang–Mills equations or the Seiberg–Witten equations. Important antecedents of Floer's work included work of Conley, Zehnder, and others on the symplectic fixed-point problem, and Witten's ideas about Morse theory.

This article describes the background material from Morse theory before discussing Floer homology of Cauchy–Riemann type and its application to the Arnol'd conjecture in symplectic topology. Floer homology in the context of four-dimensional gauge theories is discussed more briefly.

Morse Theory

Let B be a smooth, compact manifold and $f: B \rightarrow \mathbb{R}$ a smooth function. A critical point p of f is said to

be nondegenerate if the Hessian of f is a nonsingular operator on $T_p B$. The function f is a Morse function if all its critical points are nondegenerate. In the presence of a Riemannian metric g on B , the derivative df becomes a vector field, the gradient ∇f , and we can consider the downward gradient-flow equation for a path $x(s)$ in B :

$$\frac{dx}{ds} = -\nabla f(x)$$

If p and q are nondegenerate critical points, let us write $M(p, q)$ for the space of solutions $x(s)$ satisfying

$$\begin{aligned} \lim_{s \rightarrow -\infty} x(s) &= p \\ \lim_{s \rightarrow +\infty} x(s) &= q \end{aligned}$$

To understand the structure of $M(p, q)$, consider the linearization of the gradient-flow equation at a solution $x \in M(p, q)$. This is a linear equation for a vector field X along the path x in B , and takes the form

$$\nabla_{\partial/\partial s} X = -\nabla \nabla f(X) \quad [1]$$

where $\nabla \nabla f$ is the covariant derivative of the gradient ∇f , an operator on tangent vectors. Let ϵ_x be the dimension of the space of solutions X to this linear equation, with the boundary conditions $\lim_{s \rightarrow \pm\infty} X(s) = 0$, and let ϵ'_x be the dimension of the space of solutions to the adjoint equation

$$\nabla_{\partial/\partial s} X = +\nabla \nabla f(X)$$

We say that the trajectory x is “regular” if $\epsilon'_x = 0$. In this case, the trajectory space $M(p, q)$ has the structure of smooth manifold near x : its dimension is ϵ_x and its tangent space is the space of solutions X to [1]. The gradient flow is said to be Morse–Smale if all trajectories between critical points are regular. If f is any Morse function, one can always choose the metric g so that the corresponding flow is Morse–Smale. (It is also the case that one can leave g fixed and perturb f to achieve the same effect.)

In the Morse–Smale case, each $M(p, q)$ is a smooth manifold. The dimension of $M(p, q)$ in the neighborhood of a trajectory x depends only on p and q , not otherwise on x . Indeed, even without the regularity condition, the index of eqn [1], namely the difference $\epsilon_x - \epsilon'_x$, is given by

$$\epsilon_x - \epsilon'_x = \text{index}(p) - \text{index}(q)$$

where $\text{index}(p)$ denotes the number of negative eigenvalues (counting multiplicity) of the Hessian at p . In the Morse–Smale case therefore, the dimension of $M(p, q)$ is given by $\text{index}(p) - \text{index}(q)$. If $x(s)$ is a solution of the gradient-flow equation, then so is the reparametrized trajectory $x(s + c)$; and this is different from $x(s)$ as long as $p \neq q$. Let us denote by $\check{M}(p, q)$ the quotient of $M(p, q)$ by the action of \mathbb{R} given by these reparametrizations. We have

$$\dim \check{M}(p, q) = \text{index}(p) - \text{index}(q) - 1 \quad (p \neq q)$$

as long as the trajectory space is nonempty.

Let \mathbb{F}_2 denote the field with two elements. The Morse complex of a Morse–Smale gradient flow, with coefficients in \mathbb{F}_2 , is defined as follows. For each i , let $C_i(f)$ be the finite-dimensional vector space over \mathbb{F}_2 having a basis

$$e_{p_1}, \dots, e_{p_{r_i}}$$

indexed by the critical points p_1, \dots, p_{r_i} with index i . For each pair of critical points p and q with indices i and $i - 1$ respectively, let $\delta_{pq} \in \mathbb{F}_2$ denote the number of points in the zero-dimensional manifold $\check{M}(p, q)$, counted mod 2:

$$\delta_{pq} = \# \check{M}(p, q) \pmod{2}$$

The Morse–Smale condition ensures that the zero-dimensional space $\check{M}(p, q)$ is finite, so this definition is satisfactory. Define a differential

$$\delta : C_i(f) \rightarrow C_{i-1}(f)$$

by

$$\delta(e_p) = \sum_{\text{index}(q)=i-1} \delta_{pq} e_q$$

The first important fact is that δ really is a differential: as long as the flow is Morse–Smale, we have

$$\text{the composite } \delta \circ \delta : C_i(f) \rightarrow C_{i-2}(f) \text{ is zero} \quad [2]$$

We can therefore construct the homology of the complex $(C_*(f), \delta)$. This is the Morse homology:

$$H_i(f) = \frac{\ker(\delta : C_i(f) \rightarrow C_{i-1}(f))}{\text{im}(\delta : C_{i+1}(f) \rightarrow C_i(f))} \quad [3]$$

The proof of [2] is as follows. Suppose that p has index i and r is a critical point with index $i - 2$, and consider $\check{M}(p, r)$, which has dimension 1. The key step is to understand that $\check{M}(p, r)$ is noncompact, and that its ends correspond to “broken trajectories”: pairs (x_1, x_2) (modulo reparametrization), where x_1 is a gradient trajectory from p to some q of index $i - 1$, and x_2 is a trajectory from q to r . The number of ends is thus $\sum_q \delta_{pq} \delta_{rq}$. Since the number of ends of a 1-manifold is even, this sum is zero in \mathbb{F}_2 . This sum is also the matrix entry of $\delta \circ \delta$ from e_p to e_r ; so $\delta \circ \delta = 0$.

The main result about Morse homology in finite dimensions is the following:

Theorem 1 *The Morse homology $H_i(f)$ is isomorphic to the ordinary homology of the compact manifold B with coefficients \mathbb{F}_2 ; the group $H_i(B; \mathbb{F}_2)$.*

This result can be proved by first showing that $H_i(f)$ depends only on B , not on the choice of f or the metric. (This step can be accomplished by examining a nonautonomous flow of the form $dx/ds = -\nabla f(s, x)$.) Then one can examine the Morse complex in the case of a self-indexing Morse function (where the value of f at the critical points is a monotone-increasing function of their index). In the self-indexing case, the unstable manifolds of the critical points give rise to a cell decomposition of the manifold B , and the Morse complex is easily identified with the cellular chain complex for this cell decomposition.

The sum of the dimensions of the Morse homology groups cannot be larger than the sum of the dimensions of the chain groups $C_i(f)$, which is the total number of critical points. The above theorem therefore implies the following basic version of the “Morse inequalities”:

Corollary 2 *The number of critical points of a Morse function $f : B \rightarrow \mathbb{R}$ cannot be less than $\sum_i \dim H_i(B; \mathbb{F}_2)$.*

The Morse complex can be refined in various ways. For example, one can use integer coefficients in place of coefficients \mathbb{F}_2 by taking account of orientations of the spaces of trajectories. One can also introduce Morse theory with coefficients in a local system, and in both these cases a version of the above theorem continues to hold. One can also study the Morse complex of a multivalued Morse function: that is, one can start with closed 1-form α on B , with nontrivial periods, and study the flow generated by the corresponding vector field $-g^{-1}\alpha$. Such a theory was developed by Novikov.

The Morse complex can be generalized in a different direction, replacing f by a functional

related to a geometric problem. The canonical example of this (and one of the very few cases in which the theory works as in the finite-dimensional case) is the case that $B = LW$ is the space of loops $u: S^1 \rightarrow W$ in a Riemannian manifold W and f is the “energy function,” $f_E(u) = \int (du/dt)^2 dt$. If the Morse–Smale condition holds, then the Morse homology $H_i(f_E)$ computes the homology of LW , as expected. Critical points of f_E are geodesics, and the relationship between geodesics and the topology of LW , for which Corollary 2 provides a prototype, is an idea with many applications.

For the energy functional, the downward gradient-flow equation is a parabolic equation (the ordinary heat equation if the target space is Euclidean), and a solution to the flow exists for each choice of initial condition. Floer homology can be loosely characterized as the Morse theory of certain variational problems for which the gradient-flow equation is not parabolic, but elliptic of first order: the important models are the Cauchy–Riemann equation in dimension 2, the anti-self-dual Yang–Mills equations in dimension 4, or the closely related Seiberg–Witten equations. For an elliptic equation, one does not expect to solve the Cauchy problem with arbitrary initial condition; so with Floer homology, one is studying a functional for which the gradient flow is not everywhere defined. However, to define the Morse complex, the important thing is only that we have a good understanding of the trajectory spaces $M(p, q)$, which will now be solution spaces for an elliptic problem of geometric origin. The proof of Theorem 1 depends very much on the fact that the flow is everywhere defined: this theorem will therefore fail for the Morse complexes arising in Floer theory, and one must look elsewhere for a means to compute the Morse homology groups.

Before discussing Floer homology in more specific terms, we shall describe the problem in symplectic geometry that motivated its development.

The Arnol'd Conjecture

A symplectic manifold of dimension $2n$ is a smooth manifold W equipped with a 2-form ω which is closed and nondegenerate. On a symplectic manifold, one can associate to each smooth function $H: W \rightarrow \mathbb{R}$ a vector field X_H on W : the vector field is characterized by the property that

$$\omega(X_H, V) = dH(V)$$

for all vector fields V . In this situation, one refers to H as the Hamiltonian and X_H as the corresponding

Hamiltonian vector field. If W is compact, or if X_H is otherwise complete, then this vector field generates a flow $\phi_t: W \rightarrow W$ ($t \in \mathbb{R}$). We also wish to consider the case that H is time dependent: we suppose that $H_t: W \rightarrow \mathbb{R}$ is a Hamiltonian which varies smoothly with $t \in \mathbb{R}$ and is periodic, in that $H_{t+1} = H_t$. In this case, there is a time-dependent Hamiltonian vector field X_t , and we can consider the flow ϕ_t that it generates: so for $x \in W$, the path $\phi_t(x)$ will be the solution to

$$\frac{d}{dt} \phi_t(x) = X_t(x) \quad [4]$$

with initial condition $\phi_0(x) = x$. The Arnol'd conjecture, in one formulation, concerns the 1-periodic solutions to this equation, or equivalently the fixed points of $\phi_1: W \rightarrow W$. A fixed point x with $\phi_1(x) = x$ is called nondegenerate if $d\phi_1: T_x X \rightarrow T_x X$ does not have 1 as an eigenvalue. With this understood, one version of the conjecture states:

Conjecture 3 Suppose W is compact and let H_t be any 1-periodic, time-dependent Hamiltonian. If the fixed points of ϕ_1 are all nondegenerate, then the number of fixed points is not less than the sum of the Betti numbers of the manifold W .

There is another, more general version of this conjecture. Let $L \subset W$ be a closed Lagrangian submanifold: that is, an n -dimensional submanifold such that the restriction of ω to L as a 2-form is identically zero. Let $L' \subset W$ be another Lagrangian, obtained from L by a Hamiltonian isotopy: that is, L' is $\phi_1(L)$, for some flow ϕ_t generated by a time-dependent Hamiltonian H_t as above.

Question 4 If L and L' intersect transversely, is it always true that the number of intersection points of L and L' is at least the sum of the Betti numbers of the manifold L :

$$\#(L \cap L') \geq \sum_i \text{rank } H_i(L)?$$

This is phrased as a question rather than a conjecture, because the answer is certainly “no” in some cases. For example, L might be a circle contained in a small disk in a symplectic 2-manifold, in which case there is no reason why ϕ_1 should not move the disk to be completely disjoint from itself. Nevertheless, with extra hypotheses, it is known that the answer is often “yes.”

We can exhibit Conjecture 3 as a special case of Question 4, as follows. Given a symplectic manifold (V, ω) , we can form the product $W = V \times V$, with the symplectic form $\omega_W = -p_1^* \omega + p_2^* \omega$, where the p_i are the two projections. The result of this definition is

that the diagonal in $V \times V$ is a Lagrangian submanifold,

$$L \subset W = V \times V$$

for this symplectic form. Let H_t be a time-dependent Hamiltonian on V , and let $\phi_t: V \rightarrow V$ be the flow. Then $H_t \circ p_2$ is a time-dependent Hamiltonian generating a flow on W . For the flow on W , the image L' of the diagonal $L \subset W$ at time 1 is the graph of $\phi_1: V \rightarrow V$. Thus, $(L \cap L')$ can be identified with the set of fixed points of ϕ_1 in V , and an affirmative answer to Question 4 for $L \subset W$ implies Conjecture 3 for V .

Conjecture 3 and Question 4 can both be extended to the case of isolated degenerate fixed points of ϕ_1 for Conjecture 3, or to the case of isolated, nontransverse intersections for Question 4. For example, one can ask whether, in the nontransverse case, the sum of the intersection multiplicities can ever be less than the sum of the Betti numbers.

Morse Theory and the Arnol'd Conjecture

The Arnol'd conjecture, and the related Question 4, can both be studied by reformulating them as questions about the number of critical points of a carefully chosen functional.

We begin with the situation addressed by Conjecture 3. For simplicity, we suppose that $\pi_2(W)$ is zero. Let \mathcal{B} be the space of smooth, null-homotopic loops in W :

$$\mathcal{B} = \{u: S^1 \rightarrow W \mid u \text{ is smooth and null homotopic}\}$$

This is a smooth, infinite-dimensional manifold. There is a natural functional $f_0: \mathcal{B} \rightarrow \mathbb{R}$, the symplectic action, defined as

$$f_0(u) = \int_{D^2} v^*(\omega)$$

where $v: D^2 \rightarrow W$ is any extension of the map $u: S^1 \rightarrow W$. The extension v exists because u is null homotopic, and the value of f_0 is independent of the choice of v because $\pi_2(W) = 0$. This functional can be modified in the presence of a periodic Hamiltonian. Introduce a coordinate t on S^1 with period 1, and so regard u as a periodic function of t . Write the Hamiltonian as H_t as before, and define

$$f(u) = f_0(u) + \int_0^1 H_t(u(t)) dt$$

To compute the first variation of f , consider a one-parameter family of loops $u_s(t) = u(s, t)$ parametrized by $s \in \mathbb{R}$. We compute

$$\begin{aligned} \frac{d}{ds} f(u_s) &= \int_0^1 \omega\left(\frac{\partial u}{\partial s}, \frac{\partial u}{\partial t}\right) dt + \int_0^1 dH_t\left(\frac{\partial u}{\partial s}\right) dt \\ &= \int_0^1 \omega\left(\frac{\partial u}{\partial s}, \frac{\partial u}{\partial t} - X_t(u)\right) dt \end{aligned}$$

using the relationship between dH_t and X_t . Thus, a loop $u \in \mathcal{B}$ is a critical point of $f: \mathcal{B} \rightarrow \mathbb{R}$ if and only if it is a solution of the equation

$$\frac{du}{dt} = X_t(u(t)) \quad [5]$$

This means that there is a one-to-one correspondence between these critical points and certain 1-periodic solutions of eqn [4]: these in turn correspond to fixed points p of ϕ_1 with the additional property that the path $\phi_t(p)$ from p to p is null homotopic.

To consider the formal gradient flow of the functional f , one must introduce a metric on \mathcal{B} . A Riemannian metric g on the symplectic manifold (W, ω) is compatible with ω if there is an almost-complex structure $J: TW \rightarrow TW$ such that $\omega(X, Y) = g(JX, Y)$ for all tangent vectors X and Y at any point of W . Let g_t be a 1-periodic family of compatible Riemannian metrics on W . Using these, one can define an inner product on the tangent bundle of \mathcal{B} by the formula

$$\langle U, V \rangle = \int_0^1 g_t(U(t), V(t)) dt$$

in which U and V are tangent vectors at $u \in \mathcal{B}$, regarded as vector fields along the loop u in W . We can rewrite the above formula for the variation of f in terms of this inner product:

$$\left\langle \frac{\partial u}{\partial s}, J_t \left(\frac{\partial u}{\partial t} - X_t(u) \right) \right\rangle$$

where J_t is the almost-complex structure corresponding to g_t . Formally then, a one-parameter family of loops $u(s, t)$ is a solution of the downward gradient-flow equations for the functional f with respect to this metric, if u satisfies the differential equation

$$\frac{\partial u}{\partial s} + J_t \left(\frac{\partial u}{\partial t} - X_t(u) \right) = 0 \quad [6]$$

In the absence of the term X_t , and with W replaced by \mathbb{C}^n with the standard J , this equation becomes the Cauchy–Riemann equation $du/d\bar{z} = 0$, for a function u of the complex variable $z = s + it$, periodic in t .

Let us now suppose we are in the situation of Conjecture 3, so W is closed, and the fixed points of ϕ_1 are nondegenerate. As we have seen, each fixed point p of ϕ_1 corresponds to a 1-periodic solution u_p of eqn [5], a critical point of f . For each pair of fixed points p and q , introduce $M(p, q)$ as the space of solutions of the formal gradient-flow equations of f , running from p to q : that is, $M(p, q)$ is the space of maps $u: \mathbb{R} \times S^1 \rightarrow W$ satisfying eqn [6], with

$$\begin{aligned}\lim_{s \rightarrow -\infty} u(s, t) &= u_p(t) \\ \lim_{s \rightarrow +\infty} u(s, t) &= u_q(t)\end{aligned}$$

With these definitions in place, one can follow the same sequence of steps that we outlined previously in the context of finite-dimensional Morse theory, to construct the Morse complex. First, if u belongs to $M(p, q)$, we can consider the linearization at u of eqns [6], to obtain the counterpart of eqn [1]. These are linear equations for a vector field $U(s, t)$ along u in W , and take the form

$$\nabla_{\partial/\partial s} U + J_t \nabla_{\partial/\partial t} U + h(U) = 0 \quad [7]$$

where h is a linear operator of order zero. Let ϵ_u denote the dimension of the space solutions U which decay at $s = \pm\infty$, and let ϵ'_u denote the dimension of the space of solutions of the formal adjoint equation. Elliptic theory for the Cauchy–Riemann equation, and the nondegeneracy condition for u_p and u_q , mean that the operator that appears on the left-hand side of the equation is Fredholm: so both ϵ_u and ϵ'_u are finite, and the index $\epsilon_u - \epsilon'_u$ is deformation invariant. This index depends only on p and q : we give it a name,

$$\epsilon_u - \epsilon'_u = \text{index}(p, q)$$

As before, u is said to be regular if ϵ'_u is zero. For suitable choice of the almost-complex structures J_t (or equivalently the metrics g_t), the Morse–Smale condition will hold: that is, the trajectories in all spaces $M(p, q)$ are regular. In this case, each $M(p, q)$ is a smooth manifold and has dimension $\text{index}(p, q)$ if it is nonempty.

The “relative index” $\text{index}(p, q)$ plays the role of the difference of the Morse indices in the finite-dimensional case. It can be defined whether or not $M(p, q)$ is empty by considering an equation such as [7] along an arbitrary path $u(s, t)$. In general, there is no natural way to define the “index” of p : if we wish, we can select one fixed point p_0 and declare it to have index zero; we can then define $\text{index}(p)$ as $\text{index}(p, p_0)$. Alternatively, we can regard the critical points as indexed by an affine copy of \mathbb{Z} (without a preferred zero).

Imitating the construction of the Morse complex, we define a vector space CF_* over \mathbb{F}_2 as having a basis consisting of elements e_p indexed by the fixed points p . We then define $\delta: CF_* \rightarrow CF_*$ by

$$\delta e_p = \sum_{\text{index}(p, q)=1} \delta_{pq} e_q$$

where δ_{pq} is defined by counting points in $M(p, q)$ as before. The vector space CF_* is \mathbb{Z} -graded if we make a choice of critical point p_0 to have index zero; otherwise, CF_* has an “affine” \mathbb{Z} -grading. The map δ maps CF_i into CF_{i-1} .

To show that δ is well defined, and to show that $\delta \circ \delta = 0$, one must show that the zero-dimensional spaces $M(p, q)$ are compact, and that the ends of the one-dimensional spaces $M(p, r)$ correspond bijectively to broken trajectories, as in the finite-dimensional case. Both of these desired properties hold, under the Morse–Smale conditions; but this is a very special feature of the specific problem. Without the hypothesis that $\pi_2(W)$ is zero, additional noncompactness can arise from the following “bubbling” phenomenon. There could be a sequence of solutions $u^i \in M(p, q)$ to eqns [6], and a point (s_0, t_0) in $\mathbb{R} \times S^1$, such that for suitable constants ϵ_i converging to zero, the rescaled solutions

$$\tilde{u}^i(\sigma, \tau) = u^i(s_0 + \epsilon_i \sigma, t_0 + \epsilon_i \tau)$$

converge on compact subsets of the plane \mathbb{R}^2 to a nonconstant pseudoholomorphic map $\tilde{u}: \mathbb{CP}^1 \rightarrow W$, or more precisely a solution of the equation

$$\frac{\partial \tilde{u}}{\partial \sigma} + J_{t_0} \left(\frac{\partial \tilde{u}}{\partial \tau} \right) = 0$$

(In the original coordinates, the derivatives of the u^i would grow like $1/\epsilon_i$ near (s_0, t_0) .) A pseudoholomorphic sphere always has nontrivial homology class (and therefore nontrivial homotopy class); so this sort of noncompactness does not occur when $\pi_2(W) = 0$.

Granted the compactness results, the proof that $\delta \circ \delta = 0$ runs as before, and we can construct a Floer homology group,

$$HF_* = \ker(\delta) / \text{im}(\delta)$$

Unlike the Morse homology of the energy functional, the Floer homology does not yield the ordinary homology of B . To compute it, one first shows that it depends only on the symplectic manifold (W, ω) , not on the choice of Hamiltonian H_t or metrics g_t : this step is similar to the proof that the finite-dimensional Morse homology $H_*(f)$ does not depend on the Morse function. Once one has

established this independence, HF_* can be computed by examining a special case. Floer did this by taking the Hamiltonian to be independent of t and equal to a small negative multiple $-\eta h$ of a fixed Morse function $h: W \rightarrow \mathbb{R}$ on the symplectic manifold. If the multiple $\eta \in \mathbb{R}$ is small enough, the only fixed points of ϕ_1 are the stationary points of the flow, and these are exactly the critical points of h . Furthermore the only index-1 solutions of eqn [6] for small η are the solutions $u(s, t)$ with no t dependence; and these are the solutions of $du/ds = -\eta \nabla h$, the downward gradient flow of h , scaled by η . In this case therefore, the Floer complex CF_* is precisely the Morse complex $C_*(h)$ of the Morse function h , and Theorem 1 yields:

Theorem 5 *For a periodic, time-dependent Hamiltonian H_t on a closed symplectic manifold (W, ω) with $\pi_2(W) = 0$, the Floer homology HF_* is isomorphic to the ordinary homology of W with \mathbb{F}_2 coefficients, $H_*(W; \mathbb{F}_2)$.*

Because the generators of CF_* correspond to fixed points p of ϕ_1 such that the path $\phi_t(p)$ is null homotopic, the number of these fixed points is not less than the dimension of HF_* , and therefore not less than $\sum_i \dim H_i(W; \mathbb{F}_2)$ because of the above result. The sum of the mod 2 Betti numbers is at least as large as the sum of the ordinary Betti numbers (the dimensions of the rational homology groups); so one deduces, following Floer,

Corollary 6 *The Arnol'd conjecture (Conjecture 3) holds for symplectic manifolds (W, ω) satisfying the additional condition $\pi_2(W) = 0$.*

Orientations can be introduced rather as in the case of finite-dimensional Morse theory, allowing one to define Floer groups with arbitrary coefficients.

The Arnol'd conjecture is now known to hold in complete generality, without the hypothesis on π_2 . The proof has been achieved by successive extensions of the Floer homology technique. When $\pi_2(W)$ is nonzero, the space \mathcal{B} is not simply connected. The first complication that arises is that the symplectic action functional f_0 , and therefore f also, is multi-valued. This is not an obstacle initially, because ∇f is still well defined, and the spaces $M(p, q)$ of gradient trajectories can still be assumed to satisfy the Morse–Smale condition: this is the type of Morse theory considered by Novikov, as mentioned above. Because $\pi_1(\mathcal{B})$ is nontrivial, $M(p, q)$ is a union of parts $M_z(p, q)$, one for each homotopy class of paths from p to q . For each homotopy class z , we have the index $\text{index}_z(p, q)$, which is the dimension of $M_z(p, q)$.

The spaces $M_z(p, q)$ may now have additional noncompactness, due to the presence of pseudo-holomorphic spheres $\tilde{u}: \mathbb{CP}^1 \rightarrow W$. The simplest manifestation is when a sequence u^i in $M_z(p, q)$ “bubbles off” a single such sphere at a point (s_0, t_0) , and converges elsewhere to a smooth trajectory u' in $M_{z'}(p, q)$, belonging to a different homotopy class. Let σ be the homology class of the sphere \tilde{u} . Because the sphere has positive area, the pairing of σ with the de Rham class $[\omega]$ is positive: $\langle [\omega], \sigma \rangle > 0$. The indices are related by

$$\text{index}_{z'}(p, q) = \text{index}_z(p, q) - 2\langle c_1(W), \sigma \rangle$$

where $c_1(W) \in H^2(W; \mathbb{Z})$ is the first Chern class of a compatible almost-complex structure. The symplectic manifold is said to be “monotone” if, in real cohomology, $c_1(W)$ is a positive multiple of $[\omega]$. In the monotone case, we always have $\text{index}_{z'}(p, q) < \text{index}_z(p, q)$, and no bubbling off can occur for trajectory spaces $M_z(p, q)$ of index 2 or less: the above formula either makes $M_{z'}(p, q)$ a space of negative dimension (in which case it is empty) or a zero-dimensional space (in which case one has to exploit an additional transversality argument, to show that the holomorphic spheres belonging to classes σ with $\langle c_1(W), \sigma \rangle = 1$ cannot intersect one of the loops u_p in W). Since the construction of HF_* involves only the trajectories of indices 1 and 2, the construction goes through with minor changes. Because $\text{index}_z(p, q)$ depends on the path z , the group HF_* will no longer be \mathbb{Z} -graded: the grading is defined only modulo $2d$, where d is the smallest nonzero value of $\langle c_1(W), \sigma \rangle$ for spherical classes σ .

In the case that W is not monotone, additional techniques are needed to deal with the essential noncompactness of the trajectory spaces. These techniques involve (amongst other things) multi-valued perturbations on orbifolds – a strategy that requires the use of rational coefficients in order to perform the necessary averaging. For this reason, in the monotone case, the Arnol'd conjecture is known to hold only in its original form: with the ordinary (rational) Betti numbers.

To address Question 4 for Lagrangian intersections, a closely related Floer homology theory is used. Assume L is connected, and introduce the space of smooth paths joining L to L' :

$$\begin{aligned} \Omega(W; L, L') \\ = \{u: [0, 1] \rightarrow W \mid u(0) \in L, u(1) \in L'\} \end{aligned}$$

Fix a point x_0 in L , and let u_0 be the path $u_0(t) = \phi_t(x_0)$. Let \mathcal{B} be the connected component

of $\Omega(W; L, L')$ containing u_0 . On \mathcal{B} we have a symplectic action functional, defined as

$$f(u) = \int_{[0,1] \times [0,1]} v^*(\omega)$$

where $v: [0,1] \times [0,1] \rightarrow W$ is a path in \mathcal{B} with $v(0, t) = u_0(t)$ and $v(1, t) = u(t)$. The symplectic action is single valued if $\pi_2(W, L)$ is trivial (even though this condition does not guarantee that \mathcal{B} is simply connected). The critical points of f correspond to constant paths whose image in W is an intersection point of L and L' (though not all such constant paths belong to the connected component \mathcal{B}). If we fix a one-parameter family of compatible metrics g_t and almost-complex structures J_t on W , then we can consider the downward gradient trajectories of the functional. These are maps

$$u: \mathbb{R} \times [0, 1] \rightarrow W$$

satisfying the Cauchy–Riemann equation

$$\frac{\partial u}{\partial s} + J_t \left(\frac{\partial u}{\partial t} \right) = 0$$

with boundary conditions $u(s, 0) \in L$ and $u(s, 1) \in L'$. With coefficients \mathbb{F}_2 , a Morse complex can be constructed much as in the case just considered. If $\pi_2(W, L)$ is trivial, then the Floer homology group HF_* obtained as the homology of this Morse complex is isomorphic to $H_*(L; \mathbb{F}_2)$; and as a corollary, Question 4 has an affirmative answer in this case.

Without the hypothesis that $\pi_2(W, L)$ is trivial, one does not expect an affirmative answer to Question 4 in all cases. There is a “monotone” case, in which HF_* can always be defined; but it is not always isomorphic to $H_*(L; \mathbb{F}_2)$: instead, there is a spectral sequence relating the two. In the general case, there is once again the need to use rational coefficients in place of mod 2 coefficients, in order to deal with the orbifold nature of the trajectory spaces that appear. This raises the question of orientability for the trajectory spaces. In contrast to the Morse theory for Hamiltonian diffeomorphisms, there is an obstruction to orientability, involving spin structures on L and W . Even when the trajectory spaces are orientable, there are further obstructions to the existence of a Morse differential satisfying $\delta \circ \delta = 0$. The theory of these obstructions is developed in Fukaya *et al.* (2000). There are still open questions in this area.

Instanton Floer Homology

A “Floer homology theory” for 3-manifolds should assign to each 3-manifold Y (satisfying perhaps some

additional topological requirements) a group, say $\text{HF}(Y)$. Furthermore, given a four-dimensional cobordism W from Y_1 to Y_2 , the theory should provide a corresponding homomorphism of groups, from $\text{HF}(Y_1)$ to $\text{HF}(Y_2)$. These homomorphisms should satisfy the natural composition law for composite cobordisms. One can formulate this by considering the category in which an object is a closed, connected, oriented 3-manifold Y , and in which the morphisms from Y_1 to Y_2 are the oriented four-dimensional cobordisms, considered up to diffeomorphism. A Floer homology theory is then a functor from this category (perhaps with some additional decorations or restrictions) to the category of groups. Such a functor was constructed by Floer (1988a), at least for the full subcategory of homology 3-spheres (manifolds Y with $H_1 \times (Y; \mathbb{Z}) = 0$). We outline the construction.

Let $P \rightarrow Y$ be a principal $\text{SU}(2)$ bundle (necessarily trivial). Let \mathcal{A} denote the space of $\text{SU}(2)$ connections in the bundle P , and let A_0 be any chosen basepoint in \mathcal{A} . Any other $A \in \mathcal{A}$ can be written as $A_0 + a$, for some 1-form a with values in the adjoint bundle $\text{ad}(P)$ whose fiber is the Lie algebra $\mathfrak{su}(2)$. So \mathcal{A} is an affine space,

$$\mathcal{A} = A_0 + \Omega^1(Y; \text{ad}(P))$$

and we can identify the tangent space $T_A \mathcal{A}$ at any A with $\Omega^1(Y; \text{ad}(P))$. The Chern–Simons functional is a smooth function

$$\text{CS}: \mathcal{A} \rightarrow \mathbb{R}$$

depending on our choice of a reference connection A_0 . It can be defined by stating that its derivative at $A \in \mathcal{A}$ is the linear map $T_A \mathcal{A} \rightarrow \mathbb{R}$ given by

$$a \mapsto - \int_Y \text{tr}(a \wedge F_A)$$

where F_A denotes the curvature of A , as an $\text{ad}(P)$ -valued 2-form on Y , and tr denotes the trace of a matrix-valued 3-form. If we equip Y with a Riemannian metric, then we have the L^2 inner product on $\Omega^1(Y; \text{ad}(P))$, with respect to which we can consider the gradient of CS . The formal downward gradient-flow equation on \mathcal{A} is then

$$(d/ds)A = - * F_A \quad [8]$$

where $*$ is the Hodge star on Y . If $A(s)$ is a solution defined on an interval $[s_1, s_2]$, then we can form the corresponding four-dimensional connection \tilde{A} on $[s_1, s_2] \times Y$, and eqn [8] implies that \tilde{A} is a solution of the anti-self-dual Yang–Mills equation, $F_{\tilde{A}}^+ = 0$. Here $F_{\tilde{A}}^+$ is the self-dual part of the curvature 2-form on the cylinder. The critical points of CS are the flat connections on Y , with $F_A = 0$.

Let \mathcal{G} denote the gauge group, by which we mean the group of automorphisms of P . When a trivialization of P is chosen, \mathcal{G} becomes the group of smooth maps $g: Y \rightarrow \mathrm{SU}(2)$. A connection $A \in \mathcal{A}$ is irreducible if its stabilizer in \mathcal{G} consists only of the constant gauge transformations ± 1 . The functional CS is invariant only under the identity component of \mathcal{G} : it descends to a function $\mathrm{CS}: \mathcal{A}/\mathcal{G} \rightarrow \mathbb{R}/(4\pi^2\mathbb{Z})$. If we choose a basepoint in Y , then the gauge-equivalence classes of flat connections in \mathcal{A} are in one-to-one correspondence with conjugacy classes of representations,

$$\rho: \pi_1(Y) \rightarrow \mathrm{SU}(2)$$

Given representations ρ and σ , we write $M(\rho, \sigma)$ for the quotient by \mathcal{G} of the space of trajectories $A(s)$ which satisfy the gradient-flow equation [8] and which are asymptotic to flat connections belonging to the classes ρ and σ as $s \rightarrow \pm\infty$. There is a purely four-dimensional interpretation of $M(\rho, \sigma)$: it can be identified with the moduli space of solutions A to the anti-self-dual Yang–Mills equation, or “instantons,” on $\mathbb{R} \times Y$, satisfying the same asymptotic conditions.

One defines the “instanton Floer homology” of Y , roughly speaking, as the Morse homology arising from the functional CS. In the case that Y is a homology 3-sphere, Floer defined $I_*(Y)$ as the homology $H_*(C, \delta)$ of a complex C whose generators correspond to the irreducible representations ρ , and whose differential δ is defined in terms of the one-dimensional components of the moduli spaces $M(\rho, \sigma)$. To carry out the construction of $I_*(Y)$, it is necessary to perturb the functional CS to achieve a Morse–Smale condition: this is done by adding a function $f: \mathcal{A} \rightarrow \mathbb{R}$ defined in terms of the holonomy of connections along families of loops in Y . The group \mathcal{G} is not connected, and for given ρ and σ , the moduli space $M(\rho, \sigma)$ has components differing in dimension by multiples of 8. For this reason, $I_*(Y)$ is a $\mathbb{Z}/8$ -graded homology theory. It is a topological invariant of Y , and is functorial for cobordisms, in the manner outlined at the beginning of this section.

Various extensions have been made, to allow the definition of $I_*(Y)$ for 3-manifolds with nontrivial H_1 , and to incorporate the reducible representations. Although there have been some successes (Donaldson 2002), a completely satisfactory general theory has not been constructed. The main difficulties stem from the noncompactness of the instanton moduli spaces (a bubbling phenomenon) and the interaction of this bubbling with the reducible solutions.

The instanton Floer theory for 3-manifolds is closely tied up with Donaldson’s polynomial invariants of closed 4-manifolds, which are also defined using the anti-self-dual Yang–Mills equations.

Seiberg–Witten Floer Homology

Seiberg–Witten Floer homology can be defined in a manner very similar to the instanton case. Again, we start with a Riemannian 3-manifold Y , equipped now with a spin^c structure \mathfrak{s} : a rank-2 Hermitian vector bundle $S \rightarrow Y$ together with a Clifford multiplication $\rho: \Lambda^*(Y) \rightarrow \mathrm{End}(S)$. The configuration space \mathcal{C} is defined as the space of pairs (A, Φ) , where A is a spin^c connection and Φ is a section of S . In place of the Chern–Simons functional considered above, we have the Chern–Simons–Dirac functional $\mathrm{CSD}: \mathcal{C} \rightarrow \mathbb{R}$ defined by

$$\mathrm{CSD}(A, \Phi) = \frac{1}{4} \mathrm{CS}(\mathrm{tr}(A)) + \frac{1}{2} \int_Y \langle \Phi, D_A \Phi \rangle d\mu$$

where $\mathrm{tr}(A)$ denotes the connection induced by A on the line bundle $\Lambda^2 S$ and D_A is the Dirac operator for the connection A . The functional is invariant again under the identity component of the gauge group \mathcal{G} , which this time is the group of maps $g: Y \rightarrow S^1$, acting as automorphisms of S . The critical points are the solutions (A, Φ) to the three-dimensional “Seiberg–Witten equations,”

$$\begin{aligned} \frac{1}{2} \rho(F_{\mathrm{tr}(A)}) - (\Phi \Phi^*)_0 &= 0 \\ D_A \Phi &= 0 \end{aligned}$$

in which the subscript 0 denotes the traceless part of the endomorphism. If α and β are gauge-equivalence classes of critical points, then we write $M(\alpha, \beta)$ for the quotient by \mathcal{G} of the space of gradient trajectories from α to β .

As in the instanton case, $M(\alpha, \beta)$ has a four-dimensional interpretation: it is the quotient by the four-dimensional gauge group of a space of solutions (A, Φ) on $\mathbb{R} \times Y$ to the four-dimensional Seiberg–Witten equations:

$$\begin{aligned} \frac{1}{2} \rho(F_{\mathrm{tr}(A)}^+) - (\Phi \Phi^*)_0 &= 0 \\ D_A^+ \Phi &= 0 \end{aligned}$$

Here Φ is a section of the summand S^+ of the four-dimensional spin^c bundle $S = S^+ \oplus S^-$, and $D_A^+: \Gamma(S^+) \rightarrow \Gamma(S^-)$ is the four-dimensional Dirac operator.

The action of the gauge group on \mathcal{C} is free except at configurations with $\Phi = 0$. These reducible configurations have an S^1 stabilizer. Reducible critical points of CSD correspond to flat connections in the line bundle $\Lambda^2 S$. We can now distinguish two cases, according to whether $c_1(S)$ is a torsion class or not.

If $c_1(S)$ is not a torsion class, then there are no flat connections in $\Lambda^2 S$, so all critical points are irreducible. In this case, there is a straightforward Floer-type Morse theory for the functional CSD on

the space \mathcal{C}/\mathcal{G} : for generators of our complex we take the gauge-equivalence classes of critical points, and we use the one-dimensional trajectory spaces $M(\alpha, \beta)$ to define the boundary map. The resulting Morse homology group is denoted $HM_*(Y, \mathfrak{s})$. It has a canonical $\mathbb{Z}/2$ -grading, and is a topological invariant of Y and its spin^c structure.

If $c_1(S)$ is torsion, the theory is more complex. There will be reducible critical points, and one cannot exclude these from the Morse complex and still obtain a topological invariant of Y . One may incorporate the reducible critical points in two different ways, that are in a sense dual to one another; and there is a third homology theory that one can define, using the reducibles alone. Thus, one can construct three Floer groups associated to Y with the spin^c structure \mathfrak{s} . The resulting theory closely resembles the Heegaard Floer homology that is described next.

Heegaard Floer Homology and Other Floer Theories

Heegaard Floer homology is a Floer homology theory for 3-manifolds that is formally similar to Seiberg–Witten Floer homology, and conjecturally isomorphic to it. Unlike the instanton and Seiberg–Witten theories, its construction, due to Ozsváth and Szabó, does not use gauge theory. Instead, one begins with a decomposition of the 3-manifold into two handlebodies with common boundary Σ , and one studies a symplectic manifold $s^g\Sigma$, the configuration space of g -tuples of points on Σ , where g denotes the genus. The Heegaard Floer groups are then defined by a variant of the construction used for Lagrangian intersections (see the section “Morse theory and the Arnol’d conjecture”), applied to a particular pair of Lagrangian tori in $s^g\Sigma$.

As in the case of Seiberg–Witten theory, Heegaard Floer homology assigns to each oriented 3-manifold Y three different Floer groups, $HF^+(Y)$, $HF^-(Y)$, and $HF^\infty(Y)$, related by a long exact sequence:

$$\cdots \rightarrow HF^+(Y) \rightarrow HF^-(Y) \rightarrow HF^\infty(Y) \rightarrow HF^+(Y) \rightarrow \cdots$$

The first two groups are dual, in that there is a nondegenerate pairing between $HF^+(Y)$ and $HF^-(-Y)$, where $-Y$ denotes the same 3-manifold with opposite orientation. If W is an oriented four-dimensional cobordism from Y_1 to Y_2 , then there are associated functorial maps

$$\mathcal{F}^+(W) : HF^+(Y_1) \rightarrow HF^+(Y_2)$$

$$\mathcal{F}^-(W) : HF^-(Y_1) \rightarrow HF^-(Y_2)$$

$$\mathcal{F}^\infty(W) : HF^\infty(Y_1) \rightarrow HF^\infty(Y_2)$$

In addition, if the intersection form of W is not negative semidefinite, there is a map

$$\mathcal{F}(W) : HF^-(Y_1) \rightarrow HF^+(Y_2)$$

As a special case, one can start with a closed 4-manifold X , and consider the cobordism W from S^3 to S^3 obtained from X by removing two 4-balls. In this case, the map

$$\mathcal{F}(W) : HF^-(S^3) \rightarrow HF^+(S^3)$$

encodes a diffeomorphism invariant of the original 4-manifold X . This invariant is conjectured to be equivalent to the Seiberg–Witten invariants of X .

Heegaard Floer homology, and its cousin Seiberg–Witten Floer homology, have been applied successfully to settle long-standing problems in topology, particularly questions related to surgery on knots. An example of such an application is the theorem of Kronheimer *et al.* that one cannot obtain the projective space \mathbb{RP}^3 by surgery on a nontrivial knot in the 3-sphere.

In these and other applications of both Heegaard and Seiberg–Witten Floer homology, two key properties of the homology groups play an important part. The first is a nonvanishing theorem, which shows, for example, that these Floer groups can distinguish $S^1 \times S^2$ from any other manifold with the same homology. The second is a long exact sequence, which relates the Floer groups of the manifolds obtained by three different surgeries on a knot. The latter property is shared by the instanton Floer groups, as was shown by Floer (Braam and Donaldson 1995).

Other Floer-type theories have been considered, not all of which arise from a gradient flow, but in which the boundary map of the complex is obtained by counting solutions to a geometric differential equation. At the time of writing, Floer homology is an area of very active development.

See also: Four-Manifold Invariants and Physics; Gauge Theoretic Invariants of 4-Manifolds; Gauge Theory: Mathematical Applications; Knot Homologies; Ljusternik–Schnirelman Theory; Minimax Principle in the Calculus of Variations; Moduli Spaces: An Introduction; Seiberg–Witten Theory; Topological Quantum Field Theory: Overview.

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Fluid Mechanics: Numerical Methods

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The objective of this article is to give an overview of some advanced numerical methods commonly used in fluid mechanics. The focus is set primarily on finite-element methods and finite-volume methods.

Fluid Mechanics Models

Let Ω be a domain in \mathbb{R}^d ($d = 2, 3$) with boundary $\partial\Omega$ and outer unit normal \mathbf{n} . Ω is assumed to be occupied by a fluid. The basic equations governing fluid flows are derived from three conservation principles: *conservation of mass, momentum, and energy*. Denoting the density by ρ , the velocity by \mathbf{u} , and the mass specific internal energy by e_i , these equations are

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0 \quad [1]$$

$$\partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = \nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{f} \quad [2]$$

$$\partial_t (\rho e_i) + \nabla \cdot (\rho \mathbf{u} e_i) = \boldsymbol{\sigma} : \boldsymbol{\varepsilon} + q_T - \nabla \cdot \mathbf{j}_T \quad [3]$$

where $\boldsymbol{\sigma}$ is the *stress tensor*, $\boldsymbol{\varepsilon} = (1/2)(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$ is the *strain tensor*, \mathbf{f} is a body force per unit mass (gravity is a typical example), q_T is a volume source (it may model chemical reactions, Joule effects, radioactive decay, etc.), and \mathbf{j}_T is the heat flux. In addition to the above three fundamental conservation equations, one may also have to add L equations that account for the conservation of

other quantities, say ϕ_ℓ , $1 \leq \ell \leq L$. These quantities may, for example, be the concentration of constituents in an alloy, the turbulent kinetic energy, the mass fractions of various chemical species by unit volume, etc. All these conservation equations take the following form:

$$\partial_t (\rho \phi_\ell) + \nabla \cdot (\rho \mathbf{u} \phi_\ell) = q_{\phi_\ell} - \nabla \cdot \mathbf{j}_{\phi_\ell}, \quad 1 \leq \ell \leq L \quad [4]$$

Henceforth, the index ℓ is dropped to alleviate the notation.

The above set of equations must be supplemented with initial and boundary conditions. Typical initial conditions are $\rho|_{t=0} = \rho_0$, $\mathbf{u}|_{t=0} = \mathbf{u}_0$, and $\phi|_{t=0} = \phi_0$. Boundary conditions are usually classified into two types: the *essential boundary conditions* and the *natural boundary conditions*. Natural conditions impose fluxes at the boundary. Typical examples are

$$(\boldsymbol{\sigma} \cdot \mathbf{n} + \mathcal{R} \cdot \mathbf{u})|_{\partial\Omega} = \mathbf{a}_u$$

$$(\mathbf{j}_T \cdot \mathbf{n} + r_T e_i)|_{\partial\Omega} = a_T$$

and

$$(\mathbf{j}_\phi \cdot \mathbf{n} + r_\phi \phi)|_{\partial\Omega} = a_\phi$$

The quantities \mathcal{R} , r_T , r_ϕ , \mathbf{a}_u , a_T , a_ϕ are given. Essential boundary conditions consist of enforcing boundary values on the dependent variables. One typical example is the so-called *no-slip boundary condition*: $\mathbf{u}|_{\partial\Omega} = 0$.

The above system of conservation laws is closed by adding three constitutive equations whose purpose is to relate each field $\boldsymbol{\sigma}$, \mathbf{j}_T , and \mathbf{j}_ϕ to the fields ρ , \mathbf{u} , and ϕ . They account for microscopic properties of the fluid and thus must be frame-independent. Depending on the constitutive equations and

adequate hypotheses on time and space scales, various models are obtained. An important class of fluid model is one for which the stress tensor is a linear function of the strain tensor, yielding the so-called Newtonian fluid model:

$$\boldsymbol{\sigma} = (-p + \lambda \nabla \cdot \mathbf{u})\mathbf{I} + 2\mu \boldsymbol{\varepsilon} \quad [5]$$

Here p is the pressure, \mathbf{I} is the identity matrix, and λ and μ are viscosity coefficients. Still assuming linearity, common models for heat and solute fluxes consist of assuming

$$\mathbf{j}_T = -\kappa \nabla T, \quad \mathbf{j}_\phi = -D \nabla \phi \quad [6]$$

where T is the temperature. These are the so-called Fourier's law and Fick's law, respectively.

Having introduced two new quantities, namely the pressure p and the temperature T , two new scalar relations are needed to close the system. These are the state equations. One admissible assumption consists of setting $\rho = \rho(p, T)$. Another usual additional hypothesis consists of assuming that the variations in the internal energy are proportional to those in the temperature, that is, $\partial e_i = c_p \partial T$.

Let us now simplify the above models by assuming that ρ is constant. Then, mass conservation implies that the flow is incompressible, that is, $\nabla \cdot \mathbf{u} = 0$. Let us further assume that neither λ, μ , nor p depend on e_i . Then, upon abusing the notation and still denoting by p the ratio p/ρ , the above set of assumptions yields the so-called incompressible Navier–Stokes equations:

$$\nabla \cdot \mathbf{u} = 0 \quad [7]$$

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} - \nu \Delta \mathbf{u} + \nabla p = \mathbf{f} \quad [8]$$

As a result, the mass and momentum conservation equations are independent of that of the energy and those of the solutes:

$$\rho c_p (\partial_t T + \mathbf{u} \cdot \nabla T) - \nabla \cdot (\kappa \nabla T) = 2\mu \boldsymbol{\varepsilon} : \boldsymbol{\varepsilon} + q_T \quad [9]$$

$$\partial_t \phi + \mathbf{u} \cdot \nabla \phi - \frac{1}{\rho} \nabla \cdot (D \nabla \phi) = \frac{1}{\rho} q_\phi \quad [10]$$

Another model allowing for a weak dependency of ρ on the temperature, while still enforcing incompressibility, consists of setting $\rho = \rho_0(1 - \beta(T - T_0))$. If buoyancy effects induced by gravity are important, it is then possible to account for them by setting $\mathbf{f} = \rho_0 g(1 - \beta(T - T_0))$, where g is the gravitational acceleration, yielding the so-called Boussinesq model.

Variations on these themes are numerous and a wide range of fluids can be modeled by using nonlinear constitutive laws and nonlinear state laws. For the purpose of numerical simulations,

however, it is important to focus on simplified models.

The Building Blocks

From the above considerations we now extract a small set of elementary problems which constitute the building blocks of most numerical methods in fluid mechanics.

Elliptic Equations

By taking the divergence of the momentum equation [8] and assuming \mathbf{u} to be known and renaming p to ϕ , one obtains the Poisson equation

$$-\Delta \phi = f \quad [11]$$

where f is a given source term. This equation plays a key role in the computation of the pressure when solving the Navier–Stokes equations; see [54b]. Assuming that adequate boundary conditions are enforced, this model equation is the prototype for the class of the so-called elliptic equations. A simple generalization of the Poisson equation consists of the advection–diffusion equation

$$\mathbf{u} \cdot \nabla \phi - \nabla \cdot (\kappa \nabla \phi) = f \quad [12]$$

where $\kappa > 0$. Admissible boundary conditions are $(\kappa \partial_n \phi + r\phi)|_{\partial\Omega} = a$, $r \geq 0$, or $\phi|_{\partial\Omega} = a$. This type of equation is obtained by neglecting the time derivative in the heat equation [9] or in the solute conservation equation [10]. Mathematically speaking, [12] is also elliptic since its properties (in particular, the way the boundary conditions must be enforced) are controlled by the second-order derivatives. For the sake of simplicity, assume that $\mathbf{u} = 0$ in the above equation and that the boundary condition is $\phi|_{\partial\Omega} = 0$, then it is possible to show that ϕ solves [12] if and only if ϕ minimizes the functional

$$\mathcal{J}(\psi) = \int_{\Omega} (|\nabla \psi|^2 - f\psi) \, d\mathbf{x}$$

where $|\cdot|$ is the Euclidean norm and ψ spans

$$H = \left\{ \psi; \int_{\Omega} |\nabla \psi|^2 \, d\mathbf{x} < \infty; \psi|_{\partial\Omega} = 0 \right\} \quad [13]$$

Writing the first-order optimality condition for this optimization problem yields

$$\int_{\Omega} \nabla \phi \cdot \nabla \psi = \int_{\Omega} f\psi$$

for all $\psi \in H$. This is the so-called variational formulation of [12]. When \mathbf{u} is not zero, no variational principle holds but a similar way to

reformulate [12] consists of multiplying the equation by arbitrary functions in H and integrating by parts the second-order term to give

$$\int_{\Omega} (\mathbf{u} \cdot \nabla \phi) \psi + \kappa \nabla \phi \cdot \nabla \psi = \int_{\Omega} \mathbf{f} \psi, \quad \forall \psi \in H \quad [14]$$

This is the so-called weak formulation of [12]. Weak and variational formulations are the starting point for finite-element approximations.

Stokes Equations

Another elementary building block is deduced from [8] by assuming that the time derivative and the nonlinear term are both small. The corresponding model is the so-called Stokes equations,

$$-\nu \Delta \mathbf{u} + \nabla p = \mathbf{f} \quad [15]$$

$$\nabla \cdot \mathbf{u} = 0 \quad [16]$$

Assume for the sake of simplicity that the no-slip boundary condition is enforced: $\mathbf{u}|_{\partial\Omega} = 0$. Introduce the Lagrangian functional

$$\mathcal{L}(\mathbf{v}, q) = \int_{\Omega} (\nabla \mathbf{u} : \nabla \mathbf{v} - q \nabla \cdot \mathbf{v} - \mathbf{f} \cdot \mathbf{v}) \, dx$$

Set

$$X = \left\{ \mathbf{v}; \int_{\Omega} |\nabla \mathbf{v}|^2 \, dx < \infty; \mathbf{v}|_{\partial\Omega} = 0 \right\}$$

$$M = \left\{ q; \int_{\Omega} q^2 \, dx < \infty \right\}$$

Then, the pair $(\mathbf{u}, p) \in X \times M$ solves the Stokes equations if and only if it is a saddle point of \mathcal{L} , that is,

$$\mathcal{L}(\mathbf{u}, q) \leq \mathcal{L}(\mathbf{u}, p) \leq \mathcal{L}(\mathbf{v}, p), \quad \forall (\mathbf{v}, q) \in X \times M \quad [17]$$

In other words, the pressure p is the Lagrange multiplier of the incompressibility constraint $\nabla \cdot \mathbf{u} = 0$. Realizing this fact helps to understand the nature of the Stokes equations, specially when it comes to constructing discrete approximations. A variational formulation of the Stokes equations is obtained by writing the first-order optimality condition, namely:

$$\int_{\Omega} (\nu \nabla \mathbf{u} : \nabla \mathbf{v} - p \nabla \cdot \mathbf{v} - \mathbf{f} \cdot \mathbf{v}) \, dx = 0 \quad \forall \mathbf{v} \in X$$

$$\int_{\Omega} q \nabla \cdot \mathbf{u} \, dx = 0 \quad \forall q \in M$$

When the nonlinear term is not zero in the momentum equation, or when this term is linearized, there is no saddle point, but a weak formulation is obtained by multiplying the momentum

equation by arbitrary functions \mathbf{v} in X and integrating by parts the Laplacian, and by multiplying the mass equation by arbitrary functions q in M :

$$\int_{\Omega} ((\mathbf{u} \cdot \nabla \mathbf{u}) \cdot \mathbf{v} + \nu \nabla \mathbf{u} : \nabla \mathbf{v} - p \nabla \cdot \mathbf{v}) \, dx = \int_{\Omega} \mathbf{f} \cdot \mathbf{v} \quad [18]$$

$$\int_{\Omega} q \nabla \cdot \mathbf{u} \, dx = 0 \quad [19]$$

Parabolic Equations

The class of elliptic equations generalizes to that of the parabolic equations when time is accounted for:

$$\partial_t \phi + \mathbf{u} \cdot \nabla \phi - \nabla \cdot (\kappa \nabla \phi) = f, \quad \phi|_{t=0} = \phi_0 \quad [20]$$

Fundamentally, this equation has many similarities with the elliptic equation

$$\alpha \phi + \mathbf{u} \cdot \nabla \phi - \nabla \cdot (\kappa \nabla \phi) = f \quad [21]$$

where $\alpha > 0$. In particular, the set of boundary conditions that are admissible for [20] and [21] are identical, that is, it is legitimate to enforce $(\kappa \partial_n \phi + r \phi)|_{\partial\Omega} = a, r \geq 0$, or $\phi|_{\partial\Omega} = a$. Moreover, solving [21] is always a building block of any algorithm solving [20]. The important fact to remember here is that if a good approximation technique for solving [21] is at hand, then extending it to solve [20] is usually straightforward.

Hyperbolic Equations

When $\kappa/UL \rightarrow 0$, where U is the reference velocity scale and L is the reference length scale, [20] degenerates into the so-called transport equation

$$\partial_t \phi + \mathbf{u} \cdot \nabla \phi = f \quad [22]$$

This is the prototypical example for the class of hyperbolic equations. For this equation to be well-posed, it is necessary to enforce an initial condition $\phi|_{t=0} = \phi_0$ and an inflow boundary condition, that is, $\phi|_{\partial\Omega^-} = a$, where $\partial\Omega^- = \{x \in \partial\Omega; (\mathbf{u} \cdot \mathbf{n})(x) < 0\}$ is the so-called *inflow boundary* of the domain. To better understand the nature of this equation, introduce the characteristic lines $X(x, s; t)$ of $\mathbf{u}(x, t)$ defined as follows:

$$\begin{aligned} d_t X(x, s; t) &= \mathbf{u}(X(x, s; t), t) \\ X(x, s; s) &= x \end{aligned} \quad [23]$$

If \mathbf{u} is continuous with respect to t and Lipschitz with respect to \mathbf{x} , this ordinary differential equation has a unique solution. Furthermore, [22] becomes

$$d_t [\phi(X(x, s; t), t)] = f(X(x, s; t), t) \quad [24]$$

Then

$$\phi(\mathbf{x}, t) = \phi_0(\mathbf{X}(\mathbf{x}, t; 0)) + \int_0^t f(\mathbf{X}(\mathbf{x}, t; \tau), \tau) d\tau$$

provided $\mathbf{X}(\mathbf{x}, t; \tau) \in \Omega$ for all $\tau \in [0, t]$. This shows that the concept of characteristic curves is important to construct an approximation to [22].

Meshes

The starting point of every approximation technique for solving any of the above model problems consists of defining a mesh of Ω on which the approximate solution is defined. To avoid having to account for curved boundaries, let us assume that the domain Ω is a two-dimensional polygon (resp. three-dimensional polyhedron). A mesh of Ω , say \mathcal{T}_h , is a partition of Ω into small cells, hereafter assumed to be simple convex polygons in two dimensions (resp. polyhedrons in three dimensions), say triangles or quadrangles (resp. tetrahedrons or cuboids). Moreover, this partition is usually assumed to be such that if two different cells have a nonempty intersection, then the intersection is a vertex, or an entire edge, or an entire face. The left panel of Figure 1 shows a mesh satisfying the above requirement. The mesh in the right panel is not admissible.

Finite Elements: Interpolation

The finite-element method is foremost an interpolation technique. The goal of this section is to illustrate this idea by giving examples.

Let $\mathcal{T}_h = \{K_m\}_{1 \leq m \leq N_{el}}$ be a mesh composed of N_{el} simplices, that is, triangles in two dimensions or tetrahedrons in three dimensions. Consider the following vector spaces of functions:

$$V_b = \{v_b \in C^0(\bar{\Omega}); v_b|_{K_m} \in \mathbb{P}_k, 1 \leq m \leq N_{el}\} \quad [25]$$

where \mathbb{P}_k denotes the space of polynomials of global degree at most k . V_b is called a *finite-element approximation space*. We now construct a basis for V_b .

Given a simplex K_m in \mathbb{R}^d , let \mathbf{v}_n be a vertex of K_m , let F_n be the face of K_m opposite to \mathbf{v}_n , and

define \mathbf{n}_n to be the outward normal to F_n , $1 \leq n \leq d+1$. Define the *barycentric coordinates*

$$\lambda_n(\mathbf{x}) = 1 - \frac{(\mathbf{x} - \mathbf{v}_n) \cdot \mathbf{n}_n}{(\mathbf{v}_l - \mathbf{v}_n) \cdot \mathbf{n}_n}, \quad 1 \leq n \leq d+1 \quad [26]$$

where \mathbf{v}_l is an arbitrary vertex in F_n (the definition of λ_n is clearly independent of \mathbf{v}_l provided \mathbf{v}_l belongs to F_n). The barycentric coordinate λ_n is an affine function; it is equal to 1 at \mathbf{v}_n and vanishes on F_n ; its level sets are hyperplanes parallel to F_n . The barycenter of K_m has barycentric coordinates

$$\left(\frac{1}{d+1}, \dots, \frac{1}{d+1} \right)$$

The barycentric coordinates satisfy the following properties: for all $\mathbf{x} \in K_m$, $0 \leq \lambda_n(\mathbf{x}) \leq 1$, and for all $\mathbf{x} \in \mathbb{R}^d$,

$$\sum_{n=1}^{d+1} \lambda_n(\mathbf{x}) = 1 \quad \text{and} \quad \sum_{n=1}^{d+1} \lambda_n(\mathbf{x})(\mathbf{x} - \mathbf{v}_n) = 0$$

Consider the set of nodes $\{a_{n,m}\}_{1 \leq n \leq n_{sh}}$ of K_m with barycentric coordinates

$$\left(\frac{i_0}{k}, \dots, \frac{i_d}{k} \right), \quad 0 \leq i_0, \dots, i_d \leq k, \quad i_0 + \dots + i_d = k$$

These points are called the *Lagrange nodes* of K_m . It is clear that there are $n_{sh} = (1/2)(k+1)(k+2)$ of these points in two dimensions and $n_{sh} = (1/6)(k+1)(k+2)(k+3)$ in three dimensions. It is remarkable that $n_{sh} = \dim \mathbb{P}_k$.

Let $\{b_1, \dots, b_N\} = \bigcup_{K_m \in \mathcal{T}_h} \{a_{1,m}, \dots, a_{n_{sh},m}\}$ be the set of all the Lagrange nodes in the mesh. For $K_m \in \mathcal{T}_h$ and $n \in \{1, \dots, n_{sh}\}$, let $j(n, m) \in \{1, \dots, N\}$ be the integer such that $a_{n,m} = b_{j(n,m)}$; $j(n, m)$ is the global index of the Lagrange node $a_{n,m}$. Let $\{\varphi_1, \dots, \varphi_N\}$ be the set of functions in V_b defined by $\varphi_i(b_j) = \delta_{ij}$, then it can be shown that

$$\{\varphi_1, \dots, \varphi_N\} \text{ is a basis for } V_b \quad [27]$$

The functions φ_i are called *global shape functions*. An important property of global shape functions is that their supports are small sets of cells. More precisely, let $i \in \{1, \dots, N\}$ and let $\mathcal{V}_i = \{m; \exists n; i = j(n, m)\}$ be the set of cell indices to which the node b_i belongs, then the support of φ_i is $\bigcup_{m \in \mathcal{V}_i} K_m$. For $k=1$, it is clear that $\varphi_i|_{K_m} = \lambda_n$ for all $m \in \mathcal{V}_i$ and all n such that $i = j(n, m)$, and $\varphi_i|_{K_m} = 0$ otherwise. The graph of such a shape function in two dimensions is shown in the left panel of Figure 2. For $k=2$, enumerate from 1 to $d+1$ the vertices of K_m , and enumerate from $d+2$ to n_{sh} the Lagrange nodes located at the midedges. For a midedge node of index $d+2 \leq n \leq n_{sh}$, let $b(n), e(n) \in \{1, \dots, d+1\}$ be the two indices of the two Lagrange

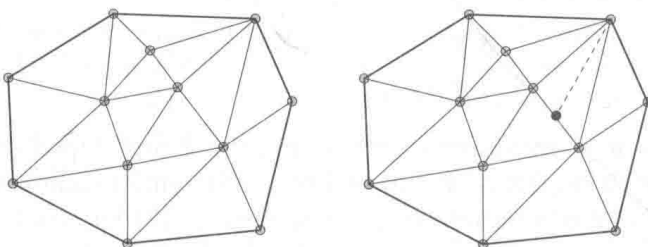


Figure 1 Admissible (left) and nonadmissible (right) meshes.

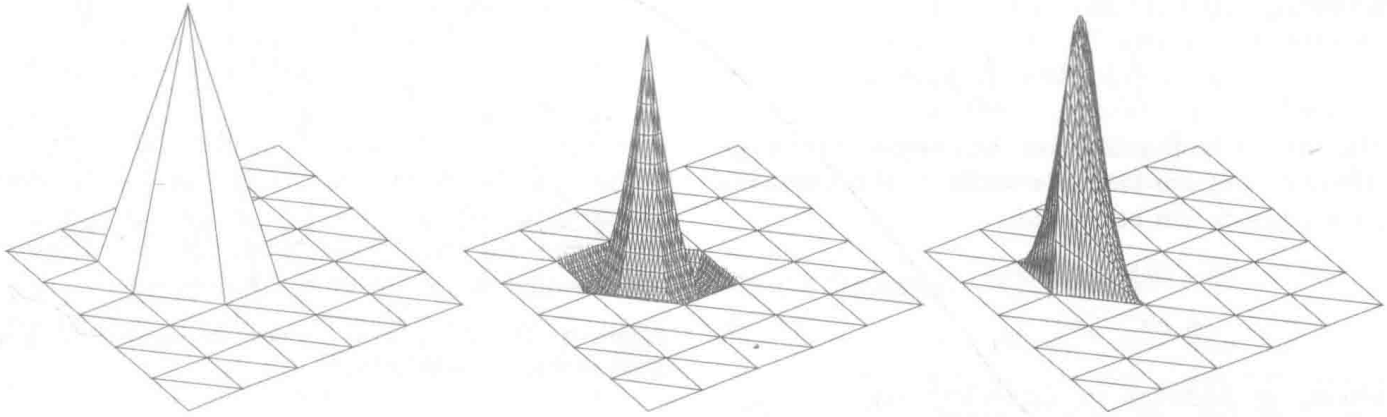


Figure 2 Two-dimensional Lagrange shape functions: piecewise P_1 (left) and piecewise P_2 (center and right).

nodes at the extremities of the edge in question. Then, the restriction to K_m of a P_2 shape function φ_i is

$$\varphi_i|_{K_m} = \begin{cases} \lambda_n(2\lambda_n - 1), & \text{if } 1 \leq n \leq d+1 \\ 4\lambda_{b(n)}\lambda_{e(n)}, & \text{if } d+2 \leq n \leq n_{sh} \end{cases} \quad [28]$$

Figure 2 shows the graph of two P_2 shape functions in two dimensions.

Once the space V_h is introduced, it is natural to define the interpolation operator

$$\Pi_h : C^0(\bar{\Omega}) \ni v \mapsto \sum_{i=1}^N v(b_i) \varphi_i \in V_h \quad [29]$$

This operator is such that for all continuous functions v , the restriction of $\Pi_h(v)$ to each mesh cell is a polynomial in P_k and $\Pi_h(v)$ takes the same values as v at the Lagrange nodes. Moreover, setting $h = \max_{K_m \in \mathcal{T}_h} \text{diam}(K_m)$, and defining

$$\|r\|_{L^p} = \left(\int_{\Omega} |r|^p dx \right)^{1/p} \quad \text{for } 1 \leq p < \infty$$

the following approximation holds:

$$\begin{aligned} \|v - \Pi_h(v)\|_{L^p} + h \|\nabla(v - \Pi_h(v))\|_{L^p} \\ \leq ch^{k+1} \|v\|_{C^{k+1}(\bar{\Omega})} \end{aligned} \quad [30]$$

where c is a constant that depends on the quality of the mesh. More precisely, for $K_m \in \mathcal{T}_h$, let ρ_{K_m} be the diameter of the largest ball that can be inscribed into K_m and let h_{K_m} be the diameter of K_m . Then, c depends on $\sigma = \max_{K_m \in \mathcal{T}_h} h_{K_m}/\rho_{K_m}$. Hence, for the mesh to have good interpolation properties, it is recommended that the cells be not too flat. Families of meshes for which σ is bounded uniformly with respect to h as $h \rightarrow 0$ are said to be *shape-regular families*.

The above example of finite-element approximation space generalizes easily to meshes composed of quadrangles or cuboids. In this case, the shape functions are piecewise polynomials of partial

degree at most k . These spaces are usually referred to as Q_k approximation spaces.

Finite Elements: Approximation

We show in this section how finite-element approximation spaces can be used to approximate some model problems exhibited in the section “Building blocks.”

Advection–Diffusion

Consider the model problem [21] supplemented with the boundary condition $(\kappa \partial_n \phi + r\phi)|_{\partial\Omega} = g$. Assume $\kappa > 0$, $\alpha + (1/2)\nabla \cdot \mathbf{u} \geq 0$, and $r \geq 0$. Define

$$\begin{aligned} a(\phi, \psi) = \int_{\Omega} ((\alpha\phi + \beta \cdot \nabla\phi)\psi + \kappa \nabla\phi \cdot \nabla\psi) dx \\ + \int_{\partial\Omega} r\phi\psi ds \end{aligned}$$

Then, the weak formulation of [21] is: seek $\phi \in H$ (H defined in [13]) such that for all $\psi \in H$

$$a(\phi, \psi) = \int_{\Omega} f\psi dx + \int_{\partial\Omega} g\psi ds \quad [31]$$

Using the approximation space V_h defined in [25] together with the basis defined in [27], we seek an approximate solution to the above problem in the form $\phi_h = \sum_{i=1}^N U_i \varphi_i \in V_h$. Then, a simple way of approximating [31] consists of seeking $U = (U_1, \dots, U_N)^T \in \mathbb{R}^N$ such that for all $1 \leq i \leq N$

$$a(\phi_h, \varphi_i) = \int_{\Omega} f\varphi_i dx + \int_{\partial\Omega} g\varphi_i ds \quad [32]$$

This problem finally amounts to solving the following linear system:

$$AU = F \quad [33]$$

where $\mathcal{A}_{ij} = a(\varphi_j, \varphi_i)$ and

$$F_i = \int_{\Omega} f \varphi_i dx + \int_{\partial\Omega} g \varphi_i ds$$

The above approximation technique is usually referred to as *the Galerkin method*. The following error estimate can be proved:

$$\begin{aligned} \|\phi - \phi_h\|_{L^p} + h \|\nabla(\phi - \phi_h)\|_{L^p} \\ \leq ch^{k+1} \|\phi\|_{C^{k+1}(\bar{\Omega})} \end{aligned} \quad [34]$$

where, in addition to depending on the shape regularity of the mesh, the constant c also depends on κ , α , and β .

Stokes Equations

The line of thought developed above can be used to approximate the Navier–Stokes problem [15]–[16]. Let us assume that the nonlinear term $\mathbf{u} \cdot \nabla \mathbf{u}$ is linearized in the form $\mathbf{v} \cdot \nabla \mathbf{u}$, where \mathbf{v} is known. Let \mathcal{T}_h be a mesh of Ω , and assume that finite-element approximation spaces have been constructed to approximate the velocity and the pressure, say X_h and M_h . Assume for the sake of simplicity that $X_h \subset X$ and $M_h \subset M$. Assume that bases for X_h and M_h are at hand, say $\{\varphi_1, \dots, \varphi_{N_u}\}$ and $\{\psi_1, \dots, \psi_{N_p}\}$, respectively. Set

$$a(\mathbf{u}, \boldsymbol{\varphi}) = \int_{\Omega} ((\mathbf{v} \cdot \nabla \mathbf{u}) \cdot \boldsymbol{\varphi} + \nu \nabla \mathbf{u} : \nabla \boldsymbol{\varphi}) dx$$

and

$$b(\mathbf{v}, \psi) = - \int_{\Omega} \psi \nabla \cdot \mathbf{v} dx$$

Then, we seek an approximate velocity $\mathbf{u}_h = \sum_{i=1}^{N_u} U_i \boldsymbol{\varphi}_i$ and an approximate pressure $p_h = \sum_{k=1}^{N_p} P_k \psi_k$ such that for all $i \in \{1, \dots, N_u\}$ and all $k \in \{1, \dots, N_p\}$ the following holds:

$$a(\mathbf{u}_h, \boldsymbol{\varphi}_i) + b(\boldsymbol{\varphi}_i, p_h) = \int_{\Omega} \mathbf{f} \cdot \boldsymbol{\varphi}_i dx \quad [35]$$

$$b(\mathbf{u}_h, \psi_k) = 0 \quad [36]$$

Define the matrix $\mathcal{A} \in \mathbb{R}^{N_u, N_u}$ such that $\mathcal{A}_{ij} = a(\boldsymbol{\varphi}_j, \boldsymbol{\varphi}_i)$. Define the matrix $\mathcal{B} \in \mathbb{R}^{N_p, N_u}$ such that $\mathcal{B}_{ki} = b(\boldsymbol{\varphi}_i, \psi_k)$. Then, the above problem can be recast into the following partitioned linear system:

$$\begin{bmatrix} \mathcal{A} & \mathcal{B}^T \\ \mathcal{B} & 0 \end{bmatrix} \begin{bmatrix} U \\ P \end{bmatrix} = \begin{bmatrix} F \\ 0 \end{bmatrix} \quad [37]$$

where the vector $F \in \mathbb{R}^{N_u}$ is such that $F_i = \int_{\Omega} \mathbf{f} \cdot \boldsymbol{\varphi}_i$.

An important aspect of the above approximation technique is that, for the linear system to be

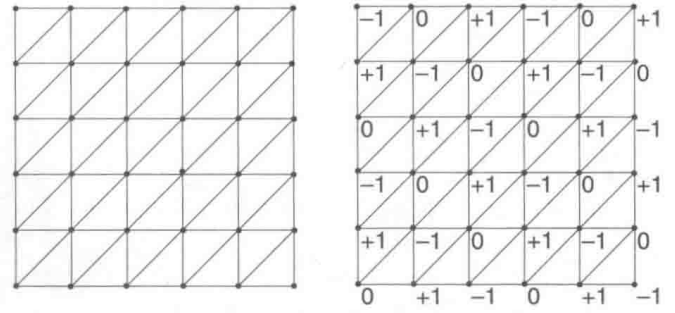


Figure 3 The P_1/P_1 finite element: the mesh (left); one pressure spurious mode (right).

invertible, the matrix \mathcal{B}^T must have full row rank (i.e., \mathcal{B} has full column rank). This amounts to

$$\exists \beta_h > 0, \quad \inf_{q_h \in M_h} \sup_{\mathbf{v}_h \in X_h} \frac{\int_{\Omega} q_h \nabla \cdot \mathbf{v}_h dx}{\|\mathbf{v}_h\|_X \|q_h\|_M} \geq \beta_h \quad [38]$$

where

$$\|\mathbf{v}_h\|_X^2 = \int_{\Omega} |\nabla \mathbf{v}_h|^2 dx, \quad \|q_h\|_M^2 = \int_{\Omega} q_h^2 dx$$

This nontrivial condition is called the *Ladyženskaja–Babuška–Brezzi condition* (LBB) in the literature. For instance, if P_1 finite elements are used to approximate both the velocity and the pressure, the above condition does not hold, since there are nonzero pressure fields q_h in M_h such that $\int_{\Omega} q_h \nabla \cdot \mathbf{v}_h dx = 0$ for all \mathbf{v}_h in X_h . Such fields are called *spurious pressure modes*. An example is shown in Figure 3. The spurious function alternatively takes the values $-1, 0$, and $+1$ at the vertices of the mesh so that its mean value on each cell is zero.

Couples of finite-element spaces satisfying the LBB condition are numerous. For instance, assuming $k \geq 2$, using P_k finite elements to approximate the velocity and P_{k-1} finite elements to approximate the pressure is acceptable. Likewise, using Q_k elements for the velocity and Q_{k-1} elements for the pressure on meshes composed of quadrangles or cuboids is admissible.

Approximation techniques for which the pressure and the velocity degrees of freedom are not associated with the same nodes are usually called *staggered approximations*. Staggering pressure and velocity unknowns is common in solution methods for the incompressible Stokes and Navier–Stokes equations; see also the subsection “Stokes equations.”

Finite Volumes: Principles

The finite-volume method is an approximation technique whose primary goal is to approximate conservation equations, whether time dependent or

not. Given a mesh, say $\mathcal{T}_h = \{K_m\}_{1 \leq m \leq N_{el}}$, and a conservation equation

$$\alpha \partial_t \phi + \nabla \cdot F(\phi, \nabla \phi, \mathbf{x}, t) = f \quad [39]$$

($\alpha = 0$ if the problem is time independent and $\alpha = 1$ otherwise), the main idea underlying every finite-volume method is to represent the approximate solution by its mean values over the mesh cells $(\phi_{K_1}, \dots, \phi_{K_{N_{el}}})^T \in \mathbb{R}^{N_{el}}$ and to test the conservation equation by the characteristic functions of the mesh cells $\{1_{K_1}, \dots, 1_{K_{N_{el}}}\}$. For each cell $K_m \in \mathcal{T}_h$, denote by \mathbf{n}_{K_m} the outward unit normal vector and denote by \mathcal{F}_m the set of the faces of K_m . The finite-volume approximation to [39] consists of seeking $(\phi_{K_1}, \dots, \phi_{K_{N_{el}}})^T \in \mathbb{R}^{N_{el}}$ such that the function $\phi_h = \sum_{m=1}^{N_{el}} \phi_{K_m} 1_{K_m}$ satisfies the following: for all $1 \leq m \leq N_{el}$

$$|K_m| \alpha d_t \phi_{K_m}(t) + \sum_{\sigma \in \mathcal{F}_m} F_b^{m,\sigma}(\phi_h, \nabla_b \phi_h, t) = \int_K f dx \quad [40]$$

where

$$|K_m| = \int_K dx$$

$\nabla_b \phi_h$ is an approximation of $\nabla \phi$, and $F_b^{m,\sigma}$ is an approximation of

$$\int_{\sigma} F(\phi, \nabla \phi, \mathbf{x}, t) \cdot \mathbf{n}_{K_m} d\sigma$$

The precise definition of the so-called approximate flux $F_b^{m,\sigma}$ depends on the nature of the problem (e.g., elliptic, parabolic, hyperbolic, saddle point) and the desired accuracy. In general, the approximate fluxes are required to satisfy the following two important properties:

1. Conservativity: for $K_m, K_l \in \mathcal{T}_h$ such that $\sigma = K_m \cap K_l$, $F_b^{m,\sigma} = -F_b^{l,\sigma}$.
2. Consistency: let ψ be the solution to [39], and set

$$\psi_h = \frac{1_{K_1}}{|K_1|} \int_{K_1} \psi dx + \dots + \frac{1_{K_{N_{el}}}}{|K_{N_{el}}|} \int_{K_{N_{el}}} \psi dx$$

then

$$F_b^{m,\sigma}(\psi_h, \nabla_b \psi_h, t) \rightarrow \int_{\sigma} F(\psi, \nabla \psi, \mathbf{x}, t) \cdot \mathbf{n} d\sigma \text{ as } h \rightarrow 0$$

The quantity

$$\left| F_b^{m,\sigma}(\psi_h, \nabla_b \psi_h, t) - \int_{\sigma} F(\psi, \nabla \psi, \mathbf{x}, t) \cdot \mathbf{n} d\sigma \right|$$

is called the consistency error.

Note that [40] is a system of ordinary differential equations. This system is usually discretized in time by using standard time-marching techniques such as explicit Euler, Runge-Kutta, etc.

The discretization technique described above is sometimes referred to as *cell-centered finite-volume method*. Another method, called *vertex-centered finite volume method*, consists of using the characteristic functions associated with the vertices of the mesh instead of those associated with the cells.

Finite Volumes: Examples

In this section we illustrate the ideas introduced above. Three examples are developed: the Poisson equation, the transport equation, and the Stokes equations.

Poisson Problem

Consider the Poisson equation [11] equipped with the boundary condition $\partial_n \phi|_{\partial\Omega} = a$. To avoid technical details, assume that $\Omega = [0, 1]^d$. Let \mathcal{K}_h be a mesh of Ω composed of rectangles (or cuboids in three dimensions).

The flux function is $F(\phi, \nabla \phi, \mathbf{x}) = -\nabla \phi$; hence, $F_b^{m,\sigma}$ must be a consistent conservative approximation of $-\int_{\sigma} \mathbf{n}_{K_m} \cdot \nabla \phi d\sigma$. Let σ be an interior face of the mesh and let K_m, K_l be the two cells such that $\sigma = K_m \cap K_l$. Let $\mathbf{x}_{K_m}, \mathbf{x}_{K_l}$ be the barycenters of K_m and K_l , respectively. Then, an admissible formula for the approximate flux is

$$F_b^{m,\sigma} = -\frac{|\sigma|}{|\mathbf{x}_{K_m} - \mathbf{x}_{K_l}|} (\phi_{K_l} - \phi_{K_m}) \quad [41]$$

where $|\sigma| = \int_{\sigma} d\sigma$. The consistency error is $\mathcal{O}(h)$ in general, and is $\mathcal{O}(h^2)$ if the mesh is composed of identical cuboids. The conservativity is evident. If σ is part of $\partial\Omega$, an admissible formula for the approximate flux is $F_b^{m,\sigma} = -\int_{\sigma} a d\sigma$. Then, upon defining $\mathcal{F}_{K_m}^i = \mathcal{F}_{K_m} \setminus \partial\Omega$ and $\mathcal{F}_{K_m}^{\partial} = \mathcal{F}_{K_m} \cap \partial\Omega$, the finite-volume approximation of the Poisson problem is: seek $\phi_h \in \mathbb{R}^{N_{el}}$ such that for all $1 \leq m \leq N_{el}$

$$\sum_{\sigma \in \mathcal{F}_{K_m}^i} F_b^{m,\sigma} = \int_{K_m} f dx + \sum_{\sigma \in \mathcal{F}_{K_m}^{\partial}} \int_{\sigma} a d\sigma \quad [42]$$

Transport Equation

Consider the transport equation

$$\partial_t \phi + \nabla \cdot (\mathbf{u} \phi) = f \quad [43]$$

$$\phi|_{t=0} = \phi_0, \quad \phi|_{\partial\Omega} = a \quad [44]$$

where $\mathbf{u}(\mathbf{x}, t)$ is a given field in $\mathcal{C}^1(\bar{\Omega} \times [0, T])$. Let \mathcal{T}_h be a mesh of Ω . For the sake of simplicity, let us use the explicit Euler time-stepping to approximate [40].

Let N be positive integer, set $\Delta t = T/N$, set $t^n = n\Delta t$ for $0 \leq n \leq N$, and partition $[0, T]$ as follows:

$$[0, T] = \bigcup_{n=0}^{N-1} [t^n, t^{n+1}]$$

Denote by $\phi_h^n \in \mathbb{R}^{N_{el}}$ the finite-volume approximation of $\phi_h(t^n)$. Then, [40] is approximated as follows:

$$\begin{aligned} & \frac{|K_m|}{\Delta t} (\phi_{K_m}^{n+1} - \phi_{K_m}^n) + \sum_{\sigma \in \mathcal{F}_m} F_b^{m,\sigma}(\phi_h, \nabla_h \phi_h, t^n) \\ &= \int_K f(x, t^n) dx \end{aligned} \quad [45]$$

where $\phi_{K_m}^0 = \int_{K_m} \phi_0 dx$. The approximate flux $F_b^{m,\sigma}$ must be a consistent conservative approximation of $\int_{\sigma} (\mathbf{u} \cdot \mathbf{n}_{K_m}) \phi d\sigma$. Let σ be a face of the mesh and let K_m, K_l be the two cells such that $\sigma = K_m \cap K_l$ (note that if σ is on $\partial\Omega$, σ belongs to one cell only and we set $K_m = K_l$). If σ is on $\partial\Omega^-$, set

$$F_b^{m,\sigma} = \int_{\sigma} (\mathbf{u} \cdot \mathbf{n}_{K_m}) a d\sigma \quad [46]$$

If σ is not on $\partial\Omega^-$, set $u_{m,\sigma}^n = \int_{\sigma} (\mathbf{u} \cdot \mathbf{n}_{K_m}) d\sigma$ and define

$$F_b^{m,\sigma} = \begin{cases} \phi_{K_m}^n u_{m,\sigma}^n & \text{if } u_{m,\sigma}^n \geq 0 \\ \phi_{K_l}^n u_{m,\sigma}^n & \text{if } u_{m,\sigma}^n < 0 \end{cases} \quad [47]$$

The above choice for the approximate flux is usually called the *upwind flux*. It is consistent with the analysis that has been done for [22], that is, information flows along the characteristic lines of the field \mathbf{u} ; see [24]. In other words, the updating of $\phi_{K_m}^{n+1}$ must be done by using the approximate values ϕ_h^n coming from the cells that are upstream the flow field.

An important feature of the above approximation technique is that it is L^∞ -stable, in the sense that

$$\max_{0 \leq n \leq N, 1 \leq m \leq N_{el}} |\phi_{K_m}^n| \leq c(u_0, f)$$

if the two mesh parameters Δt and h satisfy the so-called *Courant–Friedrichs–Levy* (CFL) condition $\|\mathbf{u}\|_{L^\infty} \Delta t / h \leq c(\sigma)$, where $c(\sigma)$ is a constant that depends on the mesh regularity parameter $\sigma = \max_{K_m \in \mathcal{T}_h} h_{K_m} / \rho_{K_m}$. In one dimension, $c(\sigma) = 1$.

Stokes Equations

To finish this short review of finite-volume methods, we turn our attention to the Stokes problem (15)–(16) equipped with the homogeneous Dirichlet boundary condition $\mathbf{u}|_{\partial\Omega} = 0$.

Let \mathcal{T}_h be a mesh of Ω composed of triangles (or tetrahedrons). All the angles in the triangulation are assumed to be acute so that, for all $K \in \mathcal{T}_h$, the intersection of the orthogonal bisectors of the sides of K , say \mathbf{x}_K , is in K . We propose a finite-volume approximation for the velocity and a finite-element approximation for the pressure. Let $\{e_1, \dots, e_d\}$ be a Cartesian basis for \mathbb{R}^d . Set $\mathbf{1}_{K_m}^k = \mathbf{1}_{K_m} e_k$ for all $1 \leq m \leq N_{el}$ and $1 \leq k \leq d$; then define

$$X_h = \text{span}\{\mathbf{1}_{K_1}^1, \dots, \mathbf{1}_{K_1}^d, \dots, \mathbf{1}_{K_{N_{el}}}^1, \dots, \mathbf{1}_{K_{N_{el}}}^d\}$$

Let $\{b_1, \dots, b_{N_v}\}$ be the vertices of the mesh, and let $\{\varphi_1, \dots, \varphi_{N_v}\}$ be the associated piecewise linear global shape functions. Then, set (see the section “Finite elements: interpolation”)

$$\begin{aligned} N_b &= \text{span}\{\varphi_1, \dots, \varphi_{N_v}\} \\ M_b &= \{q \in N_b; \int_{\Omega} q dx = 0\} \end{aligned}$$

The approximate problem consists of seeking $(\mathbf{u}_{K_1}, \dots, \mathbf{u}_{K_{N_{el}}}) \in \mathbb{R}^{dN_{el}}$ and $p_h \in M_b$ such that for all $1 \leq m \leq N_{el}$, $1 \leq k \leq d$, and all $1 \leq i \leq N_v$,

$$\sum_{\sigma \in \mathcal{F}_m} \mathbf{1}_{K_m}^k \cdot F_b^{m,\sigma} + c(\mathbf{1}_{K_m}^k, p_h) = \int_{K_m} \mathbf{1}_{K_m}^k \cdot f dx \quad [48]$$

$$c(\mathbf{u}_{K_m}, \varphi_i) = 0 \quad [49]$$

where

$$c(\mathbf{v}_{K_m}, p_h) = \int_{K_m} \mathbf{v}_{K_m} \cdot \nabla p_h dx$$

Moreover,

$$F_b^{m,\sigma} = \begin{cases} \frac{\nu|\sigma|}{|\mathbf{x}_m - \mathbf{x}_l|} (\mathbf{u}_{K_m} - \mathbf{u}_{K_l}) & \text{if } \sigma = K_m \cap K_l \\ \frac{\nu|\sigma|}{d(\mathbf{x}_m, \sigma)} \mathbf{u}_{K_m} & \text{if } \sigma = K_m \cap \partial\Omega \end{cases}$$

where $d(\mathbf{x}_{K_m}, \sigma)$ is the Euclidean distance between \mathbf{x}_{K_m} and σ . This formulation yields a linear system with the same structure as in [37]. Note in particular that

$$\sup_{\mathbf{v}_h \in X_h} \frac{c(\mathbf{v}_h, p_h)}{\|\mathbf{v}_h\|_{L^\infty}} = \|\nabla p_h\|_{L^1} \quad [50]$$

Since the mean value of p_h is zero, $\|\nabla p_h\|_{L^1}$ is a norm on M_b . As a result, an inequality similar to [38] holds. This inequality is a key step to proving that the linear system is wellposed and the approximate solution converges to the exact solution of (15)–(16).

Projection Methods for Navier–Stokes

In this section we focus on the time approximation of the Navier–Stokes problem:

$$\partial_t \mathbf{u} - \nu \Delta \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p = \mathbf{f} \quad [51a]$$

$$\nabla \cdot \mathbf{u} = 0 \quad [51b]$$

$$\mathbf{u}|_{\partial\Omega} = 0 \quad [51c]$$

$$\mathbf{u}|_{t=0} = \mathbf{u}_0 \quad [51d]$$

where \mathbf{f} is a body force and \mathbf{u}_0 is a solenoidal velocity field. There are numerous ways to discretize this problem in time, but, undoubtedly, one of the most popular strategies is to use projection methods, sometimes also referred to as *Chorin–Temam methods*.

A projection method is a fractional-step time-marching technique. It is a predictor–corrector strategy aiming at uncoupling viscous diffusion and incompressibility effects. One time step is composed of three substeps: in the first substep, the pressure is made explicit and a provisional velocity field is computed using the momentum equation; in the second substep, the provisional velocity field is projected onto the space of incompressible (solenoidal) vector fields; in the third substep, the pressure is updated.

Let $q > 0$ be an integer and approximate the time derivative of \mathbf{u} using a backward difference formula of order q . To this end, introduce a positive integer N , set $\Delta t = T/N$, set $t^n = n\Delta t$ for $0 \leq n \leq N$, and consider a partitioning of the time interval in the form

$$[0, T] = \bigcup_{n=0}^{N-1} [t^n, t^{n+1}]$$

For all sequences $\mathbf{v}_{\Delta t} = (\mathbf{v}^0, \mathbf{v}^1, \dots, \mathbf{v}^N)$, set

$$D^{(q)} \mathbf{v}^{n+1} = \beta_q \mathbf{v}^{n+1} - \sum_{j=0}^{q-1} \beta_j \mathbf{v}^{n-j} \quad [52]$$

where $q-1 \leq n \leq N-1$. The coefficients β_j are such that

$$\frac{1}{\Delta t} (\beta_q \mathbf{u}(t^{n+1}) - \sum_{j=0}^{q-1} \beta_j \mathbf{u}(t^{n-j}))$$

is a q th-order backward difference formula approximating $\partial_t \mathbf{u}(t^{n+1})$. For instance,

$$D^{(1)} \mathbf{v}^{n+1} = \mathbf{v}^{n+1} - \mathbf{v}^n$$

$$D^{(2)} \mathbf{v}^{n+1} = \frac{3}{2} \mathbf{v}^{n+1} - 2\mathbf{v}^n + \frac{1}{2} \mathbf{v}^{n-1}$$

Furthermore, for all sequences $\phi_{\Delta t} = (\phi^0, \phi^1, \dots, \phi^N)$, define

$$\phi^{*,n+1} = \sum_{j=0}^{q-1} \gamma_j \phi^{n-j} \quad [53]$$

so that $\sum_{j=0}^{q-1} \gamma_j p(t^{n-j})$ is a $(q-1)$ th-order extrapolation of $p(t^{n+1})$. For instance, $p^{*,n+1} = 0$ for $q=1$, $p^{*,n+1} = p^n$ for $q=2$, and $p^{*,n+1} = 2p^n - p^{n-1}$ for $q=3$. Finally, denote by $(\mathbf{u} \cdot \nabla \mathbf{u})^{*,n+1}$ a q th-order extrapolation of $(\mathbf{u} \cdot \nabla \mathbf{u})(t^{n+1})$. For instance,

$$(\mathbf{u} \cdot \nabla \mathbf{u})^{*,n+1} = \begin{cases} \mathbf{u}^n \cdot \nabla \mathbf{u}^n & \text{for } q=1 \\ 2\mathbf{u}^n \cdot \nabla \mathbf{u}^n - \mathbf{u}^{n-1} \cdot \nabla \mathbf{u}^{n-1} & \text{if } q=2 \end{cases}$$

A general projection algorithm is as follows. Set $\tilde{\mathbf{u}}^0 = \mathbf{u}_0$ and $\phi^l = 0$ for $0 \leq l \leq q-1$. If $q > 1$; assume that $\tilde{\mathbf{u}}^1, \dots, \tilde{\mathbf{u}}^{q-1}, p^{*,q}$ and $(\mathbf{u} \cdot \nabla \mathbf{u})^{*,q}$ have been initialized properly. For $n \geq q-1$, seek $\tilde{\mathbf{u}}^{n+1}$ such that $\tilde{\mathbf{u}}_{|\partial\Omega}^{n+1} = 0$ and

$$\begin{aligned} \frac{D^{(q)}}{\Delta t} \tilde{\mathbf{u}}^{n+1} - \nu \Delta \tilde{\mathbf{u}}^{n+1} + \nabla \left(p^{*,n+1} + \sum_{j=0}^{q-1} \frac{\beta_j}{\Delta t} \phi^{n-j} \right) \\ = \mathbf{S}^{n+1} \end{aligned} \quad [54a]$$

where $\mathbf{S}^{n+1} = \mathbf{f}(t^{n+1}) - (\mathbf{u} \cdot \nabla \mathbf{u})^{*,n+1}$. Then solve

$$\Delta \phi^{n+1} = \nabla \cdot \tilde{\mathbf{u}}^{n+1}, \quad \partial_n \phi_{|\partial\Omega}^{n+1} = 0 \quad [54b]$$

Finally, update the pressure as follows:

$$p^{n+1} = \frac{\beta_q}{\Delta t} \phi^{n+1} + p^{*,n+1} - \nu \nabla \cdot \tilde{\mathbf{u}}^{n+1} \quad [54c]$$

The algorithm [54a–c] is known in the literature as the rotational form of the pressure-correction method. Upon denoting $\mathbf{u}_{\Delta t} = (\mathbf{u}(t^0), \dots, \mathbf{u}(t^N))$ and $p_{\Delta t} = (p(t^0), \dots, p(t^N))$, the above algorithm has been proved to yield the following error estimates:

$$\|\mathbf{u}_{\Delta t} - \tilde{\mathbf{u}}_{\Delta t}\|_{\ell^2(L^2)} \leq c\Delta t^2$$

$$\|\nabla(\mathbf{u}_{\Delta t} - \tilde{\mathbf{u}}_{\Delta t})\|_{\ell^2(L^2)} + \|p_{\Delta t} - p_{\Delta t}\|_{\ell^2(L^2)} \leq c\Delta t^{3/2}$$

where $\|\phi_{\Delta t}\|_{\ell^2(L^2)}^2 = \Delta t \sum_{n=0}^N \int_{\Omega} |\phi^n|^2 dx$.

A simple strategy to initialize the algorithm consists of using $D^{(1)} \mathbf{u}^1$ at the first step in [54a]; then using $D^{(2)} \mathbf{u}^2$ at the second step, and proceeding likewise until $\tilde{\mathbf{u}}^1, \dots, \tilde{\mathbf{u}}^{q-1}$ have all been computed.

At the present time, projection methods count among the few methods that are capable of solving the time-dependent incompressible Navier–Stokes equations in three dimensions on fine meshes within reasonable

computation times. The reason for this success is that the unsplit strategy, which consists of solving

$$\frac{D^{(q)}}{\Delta t} \mathbf{u}^{n+1} - \nu \Delta \mathbf{u}^{n+1} + \nabla p^{n+1} = \mathbf{S}^{n+1} \quad [55a]$$

$$\nabla \cdot \mathbf{u}^{n+1} = 0, \quad \mathbf{u}|_{\partial\Omega}^{n+1} = 0 \quad [55b]$$

yields a linear system similar to [37], which usually takes far more time to solve than sequentially solving [54a] and [54b]. It is commonly reported in the literature that the ratio of the CPU time for solving [55a]–[55b] to that for solving [54a–c] ranges between 10 to 30.

See also: Compressible Flows: Mathematical Theory; Computational Methods in General Relativity: The Theory; Geophysical Dynamics; Image Processing: Mathematics; Incompressible Euler Equations: Mathematical Theory; Interfaces and Multicomponent Fluids; Magnetohydrodynamics; Newtonian Fluids and Thermohydraulics; Non-Newtonian Fluids; Partial Differential Equations: Some Examples; Variational Methods in Turbulence.

Fourier Law

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Introduction

In the famous 1822 treatise by Jean Baptiste Joseph Fourier, *Théorie analytique de la chaleur*, the *Discours préliminaire* opens with: “Primary causes are unknown to us; but are subject to simple and constant laws, which may be discovered by observation, the study of them being the subject of natural philosophy. Heat, like gravity, penetrates every substance of the universe, its rays occupy all parts of space. The object of our work is to set forth the mathematical laws which this element obeys. The theory of heat will hereafter form one of the most important branches of general physics.” After a brief discussion of rational mechanics, he continues with the sentence: “But whatever may be the range of mechanical theories, they do not apply to the effects of heat. These make up a special order of phenomena, which cannot be explained by the principles of motion and equilibria.” Fourier goes on with a thorough description of the phenomenology of heat transport and the derivation of the partial differential equation describing heat transport: the heat equation. A large part of the treatise is

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then devoted to solving the heat equation for various geometries and boundary conditions. Fourier’s treatise marks the birth of Fourier analysis. After Boltzmann, Gibbs, and Maxwell and the invention of statistical mechanics in the decades after Fourier’s work, we believe that Fourier was wrong and that, in principle, heat transport can and should be explained “by the principles of motion and equilibria,” that is, within the formalism of statistical mechanics. But well over a century after the foundations of statistical mechanics were laid down, we still lack a mathematically reasonable derivation of Fourier’s law from first principles. Fourier’s law describes the macroscopic transport properties of heat, that is, energy, in nonequilibrium systems. Similar laws are valid for the transport of other locally conserved quantities, for example, charge, particle density, momentum, etc. We will not discuss these laws here, except to point out that in none of these cases macroscopic transport laws have been derived from microscopic dynamics. As Peierls once put it: “It seems there is no problem in modern physics for which there are on record as many false starts, and as many theories which overlook some essential feature, as in the problem of the thermal conductivity of [electrically] non-conducting crystals.”

Macroscopic Law

Consider a macroscopic system characterized at some initial time, say $t=0$, by a nonuniform

temperature profile $T_0(\mathbf{r})$. This temperature profile will generate a heat, that is, energy current $\mathbf{J}(\mathbf{r})$. Due to energy conservation and basic thermodynamics:

$$c_v(T) \frac{\partial}{\partial t} T(\mathbf{r}, t) = -\nabla \cdot \mathbf{J} \quad [1]$$

where $c_v(T)$ is the specific heat per unit volume. On the other hand, we know that if the temperature profile is uniform, that is, if $T_0(\mathbf{r}) \equiv T_0$, there is no current in the system. It is then natural to assume that, for small temperature gradients, the current is given by

$$\mathbf{J}(\mathbf{r}) = -\kappa(T(\mathbf{r})) \nabla T(\mathbf{r}) \quad [2]$$

where $\kappa(T)$ is the conductivity. Here we have assumed that there is no mass flow or other mode of energy transport besides heat conduction (we also ignore, for simplicity, any variations in density or pressure). Equation [2] is normally called as Fourier's law. Putting together eqns [1] and [2], we get the heat equation:

$$c_v(T) \frac{\partial}{\partial t} T(\mathbf{r}, t) = \nabla \cdot [\kappa(T) \nabla T] \quad [3]$$

This equation must be completed with suitable boundary conditions. Let us consider two distinct situations in which the heat equation is observed to hold experimentally with high precision:

1. An isolated macroscopic system, for example, a fluid or solid in a domain Λ surrounded by effectively adiabatic walls. In this case, eqn [3] is to be solved subject to the initial condition $T(\mathbf{r}, 0) = T_0(\mathbf{r})$ and no heat flux across the boundary of Λ (denoted by $\partial\Lambda$), that is, $\mathbf{n}(\mathbf{r}) \cdot \nabla T(\mathbf{r}) = 0$ if $\mathbf{r} \in \partial\Lambda$ with \mathbf{n} the normal vector to $\partial\Lambda$ at \mathbf{r} . As $t \rightarrow \infty$, the system reaches a stationary state characterized by a uniform temperature \bar{T} determined by the constancy of the total energy.
2. A system in contact with heat reservoirs. Each reservoir α fixes the temperature of some portion $(\partial\Lambda)_\alpha$ of the boundary $\partial\Lambda$. The rest of the boundary is insulated. When the system reaches a stationary state (again assuming no matter flow), its temperature will be given by the solution of eqn [3] with the left-hand side set equal to zero,

$$\nabla \cdot \tilde{\mathbf{J}}(\mathbf{r}) = \nabla \cdot (\kappa \nabla \tilde{T}(\mathbf{r})) = 0 \quad [4]$$

subject to the boundary condition $\tilde{T}(\mathbf{r}) = T_\alpha$ for $\mathbf{r} \in (\partial\Lambda)_\alpha$ and no flux across the rest of the boundary.

The simplest geometry for a conducting system is that of a cylindrical slab of height h and cross-

sectional area A . It can be either a cylindrical container filled with a fluid or a piece of crystalline solid. In both cases, one keeps the lateral surface of the cylinder insulated. If the top and the bottom of the cylinder are also insulated we are in case (1). If one keeps the top and the bottom in contact with thermostats at temperatures T_h and T_b , respectively, this is (for a fluid) the usual setup for a Benard experiment. To avoid convection, one has to make $T_h > T_b$ or keep $|T_h - T_b|$ small. Assuming uniformity in the direction perpendicular to the vertical x -axis one has, in the stationary state, a temperature profile $\tilde{T}(x)$ with $\tilde{T}(0) = T_b$, $\tilde{T}(h) = T_h$ and $\kappa(\tilde{T}) d\tilde{T}/dx = \text{const.}$ for $x \in (0, h)$.

In deriving the heat equation, we have implicitly assumed that the system is described fully by specifying its temperature $T(\mathbf{r}, t)$ everywhere in Λ . What this means on the microscopic level is that we imagine the system to be in local thermal equilibrium (LTE). Heuristically, we might think of the system as being divided up (mentally) into many little cubes, each large enough to contain very many atoms yet small enough on the macroscopic scale to be accurately described, at a specified time t , as a system in equilibrium at temperature $T(\mathbf{r}_i, t)$, where \mathbf{r}_i is the center of the i th cube. For slow variation in space and time, we can then use a continuous description $T(\mathbf{r}, t)$. The theory of the heat equation is very developed and, together with its generalizations, plays a central role in modern analysis. In particular, one can consider more general boundary conditions. Here we are interested in the derivation of eqn [2] from first principles. This clearly presupposes, as a first fundamental step, a precise definition of the concept of LTE and its justification within the law of mechanics.

Empirical Argument

A theory of heat conduction has as a goal the computation of the conductivity $\kappa(T)$ for realistic models, or, at the very least, the derivation of behavior of $\kappa(T)$ as a function of T . The early analysis was based on "kinetic theory." Its application to heat conduction goes back to the works of Clausius, Maxwell, and Boltzmann, who obtained a theoretical expression for the heat conductivity of gases, $\kappa \sim \sqrt{T}$, independent of the gas density. This agrees with experiment (when the density is not too high) and was a major early achievement of the atomic theory of matter.

Heat Conduction in Gases

Clausius and Maxwell used the concept of a "mean free path" λ : the average distance a particle (atom or

molecule) travels between collisions in a gas with particle density ρ . Straightforward analysis gives $\lambda \sim 1/\rho\pi\sigma^2$, where σ an “effective” hard-core diameter of a particle. They considered a gas with temperature gradient in the x -direction and assumed that the gas is (approximately) in local equilibrium with density ρ and temperature $T(x)$. Between collisions, a particle moves a distance λ carrying a kinetic energy proportional to $T(x)$ from x to $x + \lambda/\sqrt{3}$, while in the opposite direction the amount carried is proportional to $T(x + \lambda\sqrt{3})$. Taking into account the fact that the speed is proportional to \sqrt{T} the amount of energy J transported per unit area and time across a plane perpendicular to the x -axis is approximately

$$J \sim \rho\sqrt{T} [T(x) - T(x + \lambda\sqrt{3})] \\ \sim -\sigma^{-2}\sqrt{T} \frac{dT}{dx} \quad [5]$$

and so $\kappa \sim \sqrt{T}$ independent of ρ , in agreement with experiment. It was clear to the founding fathers that starting with a local equilibrium situation the process described above will produce, as time goes on, a deviation from LTE. They reasoned, however, that this deviation from local equilibrium will be small when $(\lambda/T)dT/dx \ll 1$, the regime in which Fourier’s law is expected to hold, and the above calculation should yield, up to some factor of order unity, the right heat conductivity. To have a more precise theory, one can describe the state of the gas through the probability distribution $f(\mathbf{r}, \mathbf{p}, t)$ of finding a particle in the volume element $d\mathbf{r} d\mathbf{p}$ around the phase space point (\mathbf{r}, \mathbf{p}) . Here LTE means that

$$f(\mathbf{r}, \mathbf{p}, t) \simeq \exp\left(-\frac{p^2}{2mkT(\mathbf{r})}\right)$$

where m is the mass of the particles. If one computes the heat flux at a point \mathbf{r} by averaging the microscopic energy current at \mathbf{r} , $j = \rho\mathbf{v}(1/2mv^2)$, over $f(\mathbf{r}, \mathbf{p}, t)$ then it is only the deviation from local equilibrium which makes a contribution. The result however is essentially the same as eqn [5]. This was shown by Boltzmann, who derived an accurate formula for κ in gases by using the Boltzmann equation. If one takes κ from experiment, the above analysis yields a value for σ , the effective size of an atom or molecule, which turns out to be close to other determinations of the characteristic size of an atom. This gave an evidence for the reality of atoms and the molecular theory of heat.

Heat Conduction in Insulating Crystals

In (electrically) conducting solids, heat is mainly transported by the conduction electron. In this case, one can adapt the theory discussed in the previous

section. In (electrically) insulating solids, on the other hand, heat is transmitted through the vibrations of the lattice. In order to use the concepts of kinetic theory, it is useful to picture a solid as a gas of phonons which can store and transmit heat. A perfectly harmonic crystal, due to the fact that phonons do not interact, has an infinite thermal conductivity: in the language of kinetic theory, the mean free path λ is infinite. In a real crystal, the anharmonic forces produce interactions between the phonons and therefore a finite mean free path. Another source of finite thermal conductivity may be the lattice imperfections and impurities which scatter the phonons. Debye devised a kind of kinetic theory for phonons in order to describe thermal conductivity. One assumes that a small gradient of temperature is imposed and that the collisions between phonons maintain local equilibrium. An elementary argument gives a thermal conductivity analogous to eqn [5] obtained in the last subsection for gases (remembering, however, that the density of phonons is itself a function of T)

$$\kappa \sim c_v c^2 \tau \quad [6]$$

where, with respect to eqn [5], ρ has been replaced by c_v , the specific heat of phonons, \sqrt{T} by c , the (mean) velocity of the phonons, and λ by $c\tau$, where τ is the effective mean free time between phonon collisions. The thermal conductivity depends on the temperature via τ , and a more refined theory is needed to account for this dependence. This was done by Peierls via a Boltzmann equation for the phonons. In collisions among phonons, the momentum of phonons is conserved only modulo a vector of the reciprocal lattice. One calls “normal processes” those where the phonon momentum is conserved and “Umklap processes” those where the initial and final momenta differ by a nonzero reciprocal lattice vector. Peierls’ theory may be summarized (very roughly) as follows: in the absence of Umklap processes, the mean free path, and thus the thermal conductivity of an insulating solid, is infinite. A success of Peierls’ theory is to describe correctly the temperature dependence of the thermal conductivity. Furthermore, on the basis of this theory, one does not expect a finite thermal conductivity in one-dimensional monoatomic lattices with pair interactions. This seems so far to be a correct prediction, at least in the numerous numerical results performed on various models.

Statistical Mechanics Paradigm: Rigorous Analysis

In a rigorous approach to the above arguments, we have to first formulate precisely the problem on a

mathematical level. It is natural to adapt the standard formalism of statistical mechanics to our situation. To this end, we assume that our system is described by the positions Q and momenta P of a (very large) number of particles, N , with $Q = (q_1, \dots, q_N) \in \Lambda^N$, $\Lambda \subset \mathbb{R}^d$, and $P = (p_1, \dots, p_N) \in \mathbb{R}^{dN}$. The dynamics (in the bulk) is given by a Hamiltonian function $H(Q, P)$. A state of the system is a probability measure $\mu(P, Q)$ on phase space. As usual in statistical mechanics, the value of an observable $f(P, Q)$ will be given by the expected value of f with respect to the measure μ . In the case of a fluid contained in a region Λ , we can assume that the Hamiltonian has the form

$$\begin{aligned} H(P, Q) &= \sum_{i=1}^N \left[\frac{p_i^2}{2m} + \sum_{j \neq i} \phi(q_j - q_i) + u(q_i) \right] \\ &= \sum_{i=1}^N \frac{p_i^2}{2m} + \mathcal{V}(Q) \end{aligned} \quad [7]$$

where $\phi(q)$ is some short-range interparticle potential and $u(q_i)$ an external potential (e.g., the interaction of the particle with fixed obstacles such as a conduction electron interacting with the fixed crystalline ions). If we want to describe the case in which the temperature at the boundary is kept different in different regions $\partial\Lambda_\alpha$, we have to properly define the dynamics at the boundary of the system. A possibility is to use "Maxwell boundary conditions": when a particle hits the wall in $\partial\Lambda_\alpha$, it gets reflected and re-emerges with a distribution of velocities

$$f_\alpha(dv) = \frac{m^2}{2\pi(kT_\alpha)^2} |v_x| \exp\left[-\frac{mv^2}{2kT_\alpha}\right] dv \quad [8]$$

Several other ways to impose boundary conditions have been considered in the literature. The notion of LTE can be made precise here in the so-called hydrodynamic scaling limit (HSL), where the ratio of microscopic to macroscopic scales goes to zero. The macroscopic coordinates r and t are related to the microscopic ones q and τ , by $r = \epsilon q$ and $t = \epsilon^\alpha \tau$, that is, if Λ is a cube of macroscopic sides l , then its sides, now measured in microscopic length units, are of length $L = \epsilon^{-1}l$. We then suppose that at $t=0$ our system of $N = \rho L^d$ particles is described by an equilibrium Gibbs measure with a temperature $T(r) = T(\epsilon q)$: roughly speaking, the phase-space ensemble density has the form

$$\begin{aligned} \mu_0(P, Q) &\sim \exp\left\{-\sum_{i=1}^N \beta_0(\epsilon q_i) \right. \\ &\quad \left. \times \left[\frac{p_i^2}{2m} + \sum_{j \neq i} \phi(q_j - q_i) + u(q_i) \right] \right\} \end{aligned} \quad [9]$$

where $\beta_0^{-1}(r) = T_0(r)$. In the limit $\epsilon \rightarrow 0$, ρ fixed, the system at $t=0$ will be macroscopically in LTE with a local temperature $T_0(r)$ (as already noted, here we suppress the variation in the particle density $n(r)$). We are interested in the behavior of a macroscopic system, for which $\epsilon \ll 1$, at macroscopic times $t \geq 0$, corresponding to microscopic times $\tau = \epsilon^{-\alpha}t$, $\alpha=2$ for heat conduction or other diffusive behavior. The implicit assumption then made in the macroscopic description given earlier is that, since the variations in $T_0(r)$ are of order ϵ on a microscopic scale, then for $\epsilon \ll 1$, the system will, also at time t , be in a state very close to LTE, with a temperature $T(r, t)$ that evolves in time according to Fourier's law, eqn [1]. From a mathematical point of view, the difficult problem is to prove that the system stays in LTE for $t > 0$ when the dynamics are given by a Hamiltonian time evolution. This requires proving that the macroscopic system has some very strong ergodic properties, for example, that the only time-invariant measures locally absolutely continuous with respect to the Lebesgue measure are, for infinitely extended spatially uniform systems, of the Gibbs type. This has only been proved so far for systems evolving via stochastic dynamics (e.g., interacting Brownian particles or lattice gases). For such stochastic systems, one can sometimes prove the hydrodynamical limit and derive macroscopic transport equations for the particle or energy density and thus verify the validity of Fourier law. Another possibility, as we already saw, is to use the Boltzmann equation. Using ideas of hydrodynamical space and time scaling described earlier, it is possible to derive a controlled expansion for the solution of the stationary Boltzmann equation describing the steady state of a gas coupled to temperature reservoirs at the top and bottom. One then shows that for $\epsilon \ll 1$, ϵ being now the ratio λ/L , the Boltzmann equation for f in the slab has a time-independent solution which is close to a local Maxwellian, corresponding to LTE (apart from boundary layer terms) with a local temperature and density given by the solution of the Navier-Stokes equations which incorporates Fourier's law as expressed in eqn [2]. The main mathematical problem is in controlling the remainder in an asymptotic expansion of f in power of ϵ . This requires that the macroscopic temperature gradient, that is, $|T_1 - T_2|/h$, where $h = \epsilon L$ is the thickness of the slab on the macroscopic scale, be small. Even if this apparently technical problem could be overcome, we would still be left with the question of justifying the Boltzmann equation for such steady states and, of course, it would not tell us anything

about dense fluids or crystals. In fact, the Boltzmann equation itself is really closer to a macroscopic than to a microscopic description. It is obtained in a well-defined kinetic scaling limit in which, in addition to rescaling space and time, the particle density goes to zero, that is, $\lambda \gg \sigma$.

A simplified model of a crystal is characterized by the fact that all atoms oscillate around given equilibrium positions. The equilibrium positions can be thought of as the points of a regular lattice in \mathbb{R}^d , say \mathbb{Z}^d . Although $d=3$ is the physical situation, one can also be interested in the case $d=1,2$. In this situation, $\Lambda \subset \mathbb{Z}^d$ with cardinality N , and each atom is identified by its position $\mathbf{x}_i = \mathbf{i} + \mathbf{q}_i$, where $\mathbf{i} \in \Lambda$ and $\mathbf{q}_i \in \mathbb{R}^d$ is the displacement of the particle at lattice site \mathbf{i} from this equilibrium position. Since interatomic forces in real solids have short range, it is reasonable to assume that the atoms interact only with their nearest neighbors via a potential that depends only on the relative distance with respect to the equilibrium distance. Accordingly, the Hamiltonians that we consider have the general form

$$\begin{aligned} H(P, Q) &= \sum_{i \in \Lambda} \frac{p_i^2}{2m} + \sum_{|i-j|=1} V(\mathbf{q}_i - \mathbf{q}_j) + \sum_i U_i(\mathbf{q}_i) \\ &= \sum_{i \in \Lambda} \frac{p_i^2}{2m} + \mathcal{V}(Q) \end{aligned} \quad [10]$$

where $P = (p_i)_{i \in \Lambda}$ and analogously for Q . We shall further assume that as $|q| \rightarrow \infty$ so do $U_i(q)$ and $V(q)$. The addition of $U_i(q)$ pins down the crystal and ensures that $\exp[-\beta H(P, Q)]$ is integrable with respect to $dP dQ$, and thus the corresponding Gibbs measure is well defined. In this case, in order to fix the temperature at the boundary, one can add a Langevin term to the equation of particles on the boundaries, that is, if $\mathbf{i} \in \partial\Lambda_\alpha$ the equation for the particle is

$$\dot{p}_i = -\partial_{q_i} H(P, Q) - \lambda p_i + \sqrt{\lambda T_\alpha} \dot{w}_i \quad [11]$$

where \dot{w}_i is a standard white noise. Other thermostatting mechanisms can be considered. In this case we can also define LTE using eqn [9] but we run into the same difficulties described above – although the problem is somehow simpler due to the presence of the lattice structure and the fact that the particles oscillate close to their equilibrium points. We can obtain Fourier's law only by adding stochastic terms, for example, terms like eqn [11], to the equation of motion of every particle and assuming that $U(q)$ and $V(q)$ are harmonic. These added noises can be thought of as an effective description of the chaotic motion generated by the anharmonic terms in $U(q)$ and $V(q)$.

Just how far we are from establishing rigorously the Fourier law is clear from our very limited mathematical understanding of the stationary nonequilibrium state (SNS) of mechanical systems whose ends are, as in the example of the Benard problem, kept at fixed temperatures T_1 and T_2 . Various models have been considered, for example, models with Hamiltonian [10] coupled at the boundaries with heat reservoirs described by eqns [11]. The best mathematical results one can prove are: the existence and uniqueness of SNS; the existence of a stationary nontrivial heat flow; properties of the fluctuations of the heat flow in the SNS; the central-limit theorem type fluctuations (related to Kubo formula and Onsager relations; and large-deviation type fluctuations related to the Gallavotti–Cohen fluctuation theorem). What is missing is information on how the relevant quantities depend on the size of the system, N . In this context, the heat conductivity can be defined precisely without invoking LTE. To do this, we let \tilde{J} be the expectation value in the SNS of the energy or heat current flowing from reservoir 1 to reservoir 2. We then define the conductivity κ_L as $\tilde{J}/(A\delta T/L)$, where $\delta T/L = (T_1 - T_2)/L$ is the effective temperature gradient for a cylinder of microscopic length L and uniform cross section A , and $\kappa(T)$ is the limit of κ_L when $\delta T \rightarrow 0$ ($T_1 = T_2 = T$) and $L \rightarrow \infty$. The existence of such a limit with κ positive and finite is what one would like to prove.

See also: Dynamical Systems and Thermodynamics; Ergodic Theory; Interacting Particle Systems and Hydrodynamic Equations; Kinetic Equations; Nonequilibrium Statistical Mechanics: Dynamical Systems Approach; Nonequilibrium Statistical Mechanics: Interaction Between Theory and Numerical Simulations.

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Fourier–Mukai Transform in String Theory

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Introduction

The Fourier–Mukai transform has been introduced in the study of abelian varieties by Mukai and can be thought of as a nontrivial algebro-geometric analog of the Fourier transform. Since its original introduction, the Fourier–Mukai transform turned out to be a useful tool for studying various aspects of sheaves on varieties and their moduli spaces, and as a natural consequence, to learn about the varieties themselves. Various links between geometry and derived categories have been uncovered; for instance, Bondal and Orlov proved that Fano varieties, and certain varieties of general type, can be reconstructed from their derived categories. Moreover, Orlov proved a derived version of the Torelli theorem for K3 surfaces and also a structure theorem for derived categories of abelian varieties. Later, Kawamata gave evidence to the conjecture that two birational smooth projective varieties with trivial canonical sheaves have equivalent derived categories, which has been proved by Bridgeland in dimension 3.

The Fourier–Mukai transform also enters into string theory. The most prominent example is Kontsevich’s homological mirror-symmetry conjecture. The conjecture predicts (for mirror dual pairs of Calabi–Yau manifolds) an equivalence between the bounded derived category of coherent sheaves and the Fukaya category. The conjecture implies a correspondence between certain self-equivalences (given by Fourier–Mukai transforms) of the derived category and symplectic self-equivalences of the mirror manifold.

Besides their importance for geometrical aspects of mirror symmetry, the Fourier–Mukai transforms have also been important for heterotic string compactifications. The motivation for this came from the conjectured correspondence between the

heterotic string and F-theory, which both rely on elliptically fibered Calabi–Yau manifolds. To give evidence for this correspondence, an explicit description of stable holomorphic vector bundles was necessary and inspired a series of publications by Friedman, Morgan, and Witten. Their bundle construction relies on two geometrical objects: a hypersurface in the Calabi–Yau manifold together with a line bundle on it; more precisely, they construct vector bundles using a relative Fourier–Mukai transform.

Various aspects and refinements of this construction have been studied by now. For instance, a physical way to understand the bundle construction can be given using the fact that holomorphic vector bundles can be viewed as D-branes and that D-branes can be mapped under *T*-duality to new D-branes (of different dimensions).

We survey aspects of the Fourier–Mukai transform, its relative version and outline the bundle construction of Friedman, Morgan, and Witten. The construction has led to many new insights, for instance, the presence of 5-branes in heterotic string vacua has been understood. The construction also inspired a tremendous amount of work towards a heterotic string phenomenology on elliptic Calabi–Yau manifolds. For the many topics omitted the reader should consult the “Further reading” section.

The Fourier–Mukai Transforms

Every object E of the derived category on the product $X \times Y$ of two smooth algebraic varieties X and Y gives rise to a functor Φ^E from the bounded derived category $D(X)$ of coherent sheaves on X to the similar category on Y :

$$\Phi^E : D(X) \rightarrow D(Y)$$

$$F \mapsto \Phi^E(F) = R\hat{\pi}_*(\pi^*F \otimes E)$$

where $\pi, \hat{\pi}$ are the projections from $X \times Y$ to X and Y , respectively, and \otimes denotes the derived tensor product. $\Phi^E(F)$ is called Fourier–Mukai transform with kernel $E \in D(X \times Y)$ (in analogy

with the definition of an integral transform with kernel). Note that given a Fourier–Mukai functor Φ^E , $\Phi^E(F)$ is in general a complex having homology in several degrees even if F is a sheaf. Furthermore, a result by Orlov states that if X and Y are smooth projective varieties then any fully faithful functor $D(X) \rightarrow D(Y)$ is a Fourier–Mukai functor.

In analogy with the Fourier transform, there is a kind of “convolution product” giving the composition of two such functors. More precisely, given smooth algebraic varieties X, Y, Z , and elements $E \in D(X \times Y)$ and $G \in D(Y \times Z)$, we can define $G \circ E \in D(X \times Z)$ by

$$G \circ E = R\pi_{XZ,*}(\pi_{XY}^* E \otimes \pi_{YZ}^* G)$$

where $\pi_{XY}, \pi_{YZ}, \pi_{XZ}$ are the projections from $X \times Y \times Z$ to the pairwise products giving a natural isomorphism of functors

$$\Phi^G \circ \Phi^E = \Phi^{G \circ E}$$

Another analogy with the Fourier transform can be drawn. For this, assume that we have sheaves F and G which only have one nonvanishing Fourier–Mukai transform, the i th one $\Phi^i(F)$ (where $\Phi^i: D(X) \rightarrow \text{Coh}(Y), F \mapsto \mathcal{H}^i(\Phi^E(F))$; cf. remarks below) in the case of F , and the j th one $\Phi^j(G)$ in the case of G . Given such sheaves, there is the Parseval formula

$$\text{Ext}_X^b(F, G) = \text{Ext}_Y^{b+i-j}(\Phi^i(F), \Phi^j(G))$$

which gives a correspondence between the extensions of F, G and the extensions of their Fourier–Mukai transforms. This formula can be considered as the analog of the Parseval formula for the ordinary Fourier transform for functions on a torus.

The Parseval formula can be proved using two facts. First, for arbitrary coherent sheaves E, G the Ext groups can be computed in terms of the derived category, namely

$$\text{Ext}^i(E, G) = \text{Hom}_{D(X)}(E, G[i])$$

Second, the Fourier–Mukai transforms of F and G in the derived category $D(X)$ are given by $\Phi(F) = \Phi^i(F)[-i]$ and $\Phi(G) = \Phi^j(G)[-j]$. Since the Fourier–Mukai transform is an equivalence of categories, we have

$$\text{Hom}_{D(X)}(F, G[i]) = \text{Hom}_{D(X)}(\Phi^i(F), \Phi^j(G)[i-j+h])$$

implying the Parseval formula.

A first simple example of a Fourier–Mukai functor can be given: let F be the complex in $D(X \times X)$ defined by the structure sheaf \mathcal{O}_Δ of the diagonal

$\Delta \subset X \times X$. Then it is easy to check that $\Phi^F: D(X) \rightarrow D(X)$ is isomorphic to the identity functor on $D(X)$. Moreover, if we shift degrees by n taking $F = \mathcal{O}_\Delta[n]$ (a complex with only the sheaf \mathcal{O}_Δ placed in degree n), then $\Phi^F: D(X) \rightarrow D(X)$ is the degree shifting functor $\mathcal{G} \mapsto \mathcal{G}[n]$.

As we will be interested in relative Fourier–Mukai transforms for elliptic fibrations, let us consider the case of a Fourier–Mukai transform on an elliptic curve: consider an elliptic curve E with a fixed origin p_0 and identify E with $\hat{E} = \text{Pic}^0(E)$ via $f: E \rightarrow \hat{E}, x \mapsto \mathcal{O}_E(x - p_0)$. As kernel we take the normalized Poincaré line bundle $\mathcal{P} := \mathcal{O}_{E \times E}(\Delta - \{p_0\} \times E - E \times \{p_0\})$. The restriction of \mathcal{P} to $p_0 \times E$ or $E \times p_0$ is isomorphic to the trivial line bundle \mathcal{O} . \mathcal{P} has the universal property which can be expressed by $\Phi^{\mathcal{P}}(k(x)) = f(x)$, where $k(x)$ is the sheaf supported at a point $x \in E$; in particular, $\Phi^{\mathcal{P}}(k(p_0)) = \mathcal{O}_E$ and $\Phi^{\mathcal{P}}(\mathcal{O}_E) = k(p_0)[-1]$, where \mathcal{O}_E is the structure sheaf of E .

Relative Fourier–Mukai Transforms for Elliptic Fibrations

It is often convenient to study problems for families rather than for single varieties. The main advantage of the relative setting is that base-change properties (or parameter dependencies) are better encoded into the problem. We can do that for Fourier–Mukai functors as well. To this end, we consider two morphisms $p: X \rightarrow B, \hat{p}: \hat{X} \rightarrow B$ of algebraic varieties. We will assume that the morphisms are flat and so give nice families of algebraic varieties. We shall define relative Fourier–Mukai functors in this setting by means of a “kernel” E in the derived category $D(X \times_B \hat{X})$.

Let us make the relative setting explicit for elliptic fibrations: an elliptic fibration is a proper flat morphism $p: X \rightarrow B$ of schemes whose fibers are Gorenstein curves of arithmetic genus 1. We also assume that p has a section $\sigma: B \hookrightarrow X$ taking values in the smooth locus $X' \rightarrow B$ of p . The generic fibres are then smooth elliptic curves, whereas some singular fibers are allowed. If the base B is a smooth curve, elliptic fibrations were studied and classified by Kodaira, who described all the types of singular fibers that may occur, the so-called Kodaira curves. When the base is a smooth surface, more complicated configuration of singular curves can occur and have indeed been studied by Miranda.

First let us fix notation and setup. We denote by $\sigma = \sigma(B)$ the image of the section, by X_t the fiber of p over $t \in B$ (we assume, in what follows, B is either a smooth curve or surface) and by $i_t: X_t \hookrightarrow X$ the inclusion. Furthermore, $\omega_{X/B}$ is the relative dualizing

sheaf and $\omega = R^1 p_* \mathcal{O}_X \simeq (p_* \omega_{X/B})^*$, where the isomorphism is Grothendieck–Serre duality for p . The sheaf $\mathcal{L} = p_* \omega_{X/B}$ is a line bundle whose first Chern class we denote by $K = c_1(\mathcal{L})$. The adjunction formula for $\sigma \hookrightarrow X$ gives that $\sigma^2 = -\sigma \cdot p^* K$ as cycles on X . Moreover, we will consider elliptic fibrations with a section whose fibers are all geometrically integral. This means that the fibration is isomorphic with its Weierstrass model.

From Kodaira’s classification of possible singular fibers one finds that the components of reducible fibers of p which do not meet σ form rational double point configurations disjoint from σ . Let $X \rightarrow \bar{X}$ be the result of contracting these configurations and let $\bar{p}: \bar{X} \rightarrow B$ be the induced map. Then all fibers of \bar{p} are irreducible with at worst nodes or cusps as singularities. In this case, one refers to \bar{X} as the Weierstrass model of X .

The Weierstrass model can be constructed as follows: the divisor 3σ is relatively ample and, if $\mathcal{E} = p_* \mathcal{O}_X(3\sigma) \simeq \mathcal{O}_B \oplus \omega^{\otimes 2} \oplus \omega^{\otimes 3}$ and $\bar{p}: P = \mathbb{P}(\mathcal{E}^*) \rightarrow B$ is the associated projective bundle, there is a projective morphism $j: X \rightarrow P$ such that $j(X) = \bar{X}$.

Now special fibers of $X \rightarrow B$ can have at most one singular point, either a cusp or a simple node. Thus, in this case 3σ is relatively very ample and gives rise to a closed immersion $j: X \hookrightarrow P$ such that $j^* \mathcal{O}_P(1) = \mathcal{O}_X(3\sigma)$, where j is locally a complete intersection whose normal sheaf is $\mathcal{N}(X/P) \simeq \pi^* \omega^{-\otimes 6} \otimes \mathcal{O}_X(9\sigma)$. This follows by relative duality since $\omega_{P/B} = \bigwedge \Omega_{P/B} \simeq \pi^* \omega^{\otimes 5}(-3)$, due to the Euler exact sequence

$$0 \rightarrow \Omega_{P/B} \rightarrow \pi^* \mathcal{E}(-1) \rightarrow \mathcal{O}_P \rightarrow 0$$

The morphism $p: X \rightarrow B$ is then a local complete intersection morphism (cf. Fulton (1984)) and has a virtual relative tangent bundle $T_{X/B} = [j^* T_{P/B}] - [\mathcal{N}_{X/P}]$ in the K -group $K^*(X)$. The Todd class of $T_{X/B}$ is given by

$$\mathrm{Td}(T_{X/B}) = 1 - \frac{1}{2} p^{-1} K + \frac{1}{12} (12\sigma \cdot p^{-1} K + 13p^{-1} K^2) - \frac{1}{2} \sigma \cdot p^{-1} K^2 + \text{terms of higher degree}$$

Now if $\hat{p}: \hat{X} \rightarrow B$ denotes the dual elliptic fibration, defined as the relative moduli space of torsion-free rank-1 sheaves of relative degree 0, it is known that for $t \in B$ there is an isomorphism $\hat{X}_t \cong X_t$ between the fibers of both fibrations. Since we assume that the original fibration $p: X \rightarrow B$ has a section σ , then p and \hat{p} are globally isomorphic; hereafter we identify $X \cong \hat{X}$, where \hat{X} denotes the compactified relative Jacobian of X .

Note that \hat{X} is the scheme representing the functor which, to any scheme morphism $\phi: S \rightarrow B$, associates the space of equivalence classes of S -flat

sheaves on $p_S: X \times_B S \rightarrow S$, whose restrictions to the fibers of ϕ are torsion-free (the usual definition of “torsion free” is only for integral varieties, i.e., varieties whose local rings have no zero-divisors. In this case, a sheaf M is torsion free if for any open subset U , any nonzero section m of M on U and any nonzero section a of the relevant functions sheaf, one has $a \cdot m \neq 0$. When the variety is not integral (it is reducible, or nonreduced) this definition has no real meaning, then what substitutes the notion of “torsion free” is the Simpson definition of “pure of maximal dimension”: a sheaf M is “torsion free” in this sense if the support of any of its subsheaves is the whole variety (cf. Huybrechts and Lehn (1997)), of rank 1 and degree 0; two such sheaves $\mathcal{F}, \mathcal{F}'$ are considered to be equivalent if $\mathcal{F}' \cong \mathcal{F} \otimes p_S^* \mathcal{L}$ for a line bundle \mathcal{L} on S (cf. Altman and Kleiman (1980); note the Altman–Kleiman compactification of the relative Jacobian applies to our situation since we consider elliptic fibrations with integral fibers). Moreover, the natural morphism $X \rightarrow \hat{X}, x \mapsto \mathcal{I}_x \otimes \mathcal{O}_{X_t}(\sigma(t))$ is an isomorphism (of B -schemes); here \mathcal{I}_x is the ideal sheaf of the point x in X_t .

Note also that if $\pi: Y \rightarrow X_t$ is the normalization of one of our fibers X_t and z is the exceptional divisor (the pre-image of the singular point x) then $\pi_*(\mathcal{O}_Y(-z))$ is the maximal ideal of x .

The variety \hat{X} is a fine moduli space. This means that there exists a coherent sheaf \mathcal{P} on $X \times_B \hat{X}$ flat over \hat{X} , whose restrictions to the fibers of \hat{p} are torsion free, and of rank 1 and degree 0. The sheaf \mathcal{P} is defined, up to tensor product, by the pullback of a line bundle on \hat{X} , and is called the universal Poincaré sheaf, which we will normalize by letting $\mathcal{P}|_{\sigma \times_B \hat{X}} \simeq \mathcal{O}_X$. We shall henceforth assume that \mathcal{P} is normalized in this way, so that

$$\mathcal{P} = \mathcal{I}_\Delta \otimes \pi^* \mathcal{O}_X(\sigma) \otimes \hat{\pi}^* \mathcal{O}_X(\sigma) \otimes q^* \omega^{-1}$$

where $\pi, \hat{\pi}$ and $q = p \circ \pi = \hat{p} \circ \hat{\pi}$ refer to the diagram

$$\begin{array}{ccc} X \times_B X & \xrightarrow{\hat{\pi}} & X \\ \pi \downarrow & q \searrow & \downarrow \hat{p} \\ X & \xrightarrow{p} & B \end{array}$$

and \mathcal{I}_Δ is the ideal sheaf of the diagonal immersion $X \hookrightarrow X \times_B X$.

Starting with the diagram and with the kernel given by the normalized relative universal Poincaré sheaf \mathcal{P} on the fibered product $X \times_B X$, we define the relative Fourier–Mukai transform as

$$\begin{aligned} \Phi &= \Phi^{\mathcal{P}}: D(X) \rightarrow D(X) \\ F &\mapsto \Phi(F) = R\hat{\pi}_*(\pi^* F \otimes \mathcal{P}) \end{aligned}$$

Note that $\Phi(F)$ can be generalized if we allow changes in the base space B , that is, we consider base-change morphisms $g: S \rightarrow B$.

We close this section with some remarks:

- An important feature of Fourier–Mukai functors is that they are exact as functors of triangulated categories. In more familiar terms, we can say that for any exact sequence $0 \rightarrow \mathcal{N} \rightarrow \mathcal{F} \rightarrow \mathcal{G} \rightarrow 0$ of coherent sheaves in X , we obtain an exact sequence

$$\begin{aligned} \cdots \rightarrow \Phi^{i-1}(\mathcal{G}) \rightarrow \Phi^i(\mathcal{N}) \rightarrow \Phi^i(\mathcal{F}) \rightarrow \Phi^i(\mathcal{G}) \rightarrow \\ \Phi^{i+1}(\mathcal{N}) \rightarrow \cdots \end{aligned}$$

where we have written $\Phi = \Phi^E$ and $\Phi^i(F) = \mathcal{H}^i(\Phi(F))$ denotes the i th cohomology sheaves of the complexes $\Phi(F)$.

Given a Fourier–Mukai functor Φ^E , a complex F in $D(X)$ satisfies the WIT_i condition (or is WIT_i) if there is a coherent sheaf \mathcal{G} on \hat{X} such that $\Phi^E(F) \simeq \mathcal{G}[i]$ in $D(\hat{X})$, where $\mathcal{G}[i]$ is the associated complex concentrated in degree i . Furthermore, we say that F satisfies the IT_i condition if, in addition, \mathcal{G} is locally free.

When the kernel E is simply a sheaf \mathcal{Q} on $X \times \hat{X}$ flat over \hat{X} , the cohomology and base-change theorem (cf. Hartshorne (1977)) allows one to show that a coherent sheaf \mathcal{F} on X is IT_i if and only if $H^i(X, \mathcal{F} \otimes \mathcal{Q}_\xi) = 0$ for all $\xi \in \hat{X}$ and for all $j \neq i$, where \mathcal{Q}_ξ denotes the restriction of \mathcal{Q} to $X \times \{\xi\}$ and \mathcal{F} is WIT_0 if and only if it is IT_0 .

The acronym “IT” stands for “index theorem,” while “W” stands for “weak.” This terminology comes from Nahm transforms for connections on tori in complex differential geometry.

- The Parseval formula for the relative Fourier–Mukai transform has been proved by Mukai in his original Fourier–Mukai transform for abelian varieties and can be extended to any situation in which a Fourier–Mukai transform is fully faithful.
- For physical applications, it is often convenient to work in cohomology $H^*(X, \mathbb{Q})$. The passage from $D(X)$ to $H^*(X, \mathbb{Q})$ can be described as follows. We first send a complex $Z \in D(X)$ to its natural class in the K -group; we then make use of the fact that the Chern character ch maps $K(X) \rightarrow \text{CH}^*(X) \otimes \mathbb{Q}$ and finally we apply the cycle map to $H^*(X, \mathbb{Q})$. This passage (by abuse of notation) is often denoted by $\text{ch}: D(X) \rightarrow H^{\text{even}}(X, \mathbb{Q})$, it commutes with pullbacks and transforms tensor products into dot products. Moreover, if we substitute the Mukai vector $v(Z) = \text{ch}(Z) \sqrt{\text{Td}(X)}$ for the Chern character $\text{ch}(Z)$ then we find the commutative

diagram

$$\begin{array}{ccc} D(X) & \xrightarrow{\Phi^E} & D(Y) \\ \downarrow v & & \downarrow v \\ H^*(X, \mathbb{Q}) & \xrightarrow{\Phi^*(E)} & H^*(Y, \mathbb{Q}) \end{array}$$

This can be shown using the Grothendieck–Riemann–Roch theorem and the fact that the power series defining the Todd class starts with constant term 1 and thus is invertible.

Vector Bundles for Heterotic Strings

A compactification of the ten-dimensional heterotic string is given by a holomorphic, stable G -bundle V (with G some Lie group specified below) over a Calabi–Yau manifold X . The Calabi–Yau condition, the holomorphy and stability of V are a direct consequence of the required supersymmetry in the uncompactified spacetime. We assume that the underlying ten-dimensional space M_{10} is decomposed as $M_{10} = M_4 \times X$, where M_4 (the uncompactified spacetime) denotes the four-dimensional Minkowski space and X a six-dimensional compact space given by a Calabi–Yau 3-fold. To be more precise: supersymmetry requires that the connection A on V satisfies

$$F_A^{2,0} = F_A^{0,2} = 0, \quad F^{1,1} \wedge J^2 = 0$$

where J denotes a Kähler form of X . It follows that the connection has to be a holomorphic connection on a holomorphic vector bundle and, in addition, satisfies the Donaldson–Uhlenbeck–Yau equation, which has a unique solution if and only if the vector bundle is polystable.

In addition to X and V , we have to specify a B -field on X of field strength H . In order to get an anomaly-free theory, the Lie group G is fixed to be either $E_8 \times E_8$ or $\text{Spin}(32)/\mathbb{Z}_2$ or one of their subgroups and H must satisfy the identity

$$dH = \text{tr } R \wedge R - \text{Tr } F \wedge F$$

where R and F are, respectively, the associated curvature forms of the spin connection on X and the gauge connection on V . Also tr refers to the trace of the composite endomorphism of the tangent bundle to X and Tr denotes the trace in the adjoint representation of G . For any closed four-dimensional submanifold X_4 of the ten-dimensional spacetime M_{10} , the 4-form $\text{tr } R \wedge R - \text{Tr } F \wedge F$ must have trivial cohomology. Thus, a necessary topological condition V has to satisfy is $\text{ch}_2(TX) = \text{ch}_2(V)$, which simplifies to $c_2(TX) = c_2(V)$ for Calabi–Yau manifolds, V being an $\text{SU}(n)$ vector bundle.

A physical interpretation of the third Chern class can be given as a result of the decomposition of the ten-dimensional spacetime into a four-dimensional flat Minkowski space and X . The decomposition of the corresponding ten-dimensional Dirac operator with values in V shows that massless four-dimensional fermions are in one-to-one correspondence with zero modes of the Dirac operator D_V on X . The index of D_V can be effectively computed using the Hirzebruch–Riemann–Roch theorem and is given by

$$\text{index}(D) = \int_X \text{Td}(X) \text{ch}(V) = \frac{1}{2} \int_X c_3(V)$$

equivalently, we can write the index as $\text{index}(D) = \sum_{i=0}^3 (-1)^i \dim H^i(X, V)$. For stable vector bundles, we have $H^0(X, V) = H^3(X, V) = 0$ and so the index computes the net number of fermion generations N_{gen} in the respective model.

Now it has been observed that the inclusion of background 5-branes changes the anomaly constraint. Various 5-brane solutions of the heterotic string equations of motion have been discussed in the gauge 5-brane, the symmetric 5-brane, and the neutral 5-brane. It has been shown that the gauge and symmetric 5-brane solutions involve finite-size instantons of an unbroken nonabelian gauge group. In contrast, the neutral 5-branes can be interpreted as zero-size instantons of the $\text{SO}(32)$ heterotic string. The magnetic 5-brane contributes a source term to the Bianchi identity for the 3-form H ,

$$dH = \text{tr } R \wedge R - \text{Tr } F \wedge F + n_5 \sum_{\text{five-branes}} \delta_5^{(4)}$$

and integration over a 4-cycle in X gives the anomaly constraint

$$c_2(TX) = c_2(V) + [W]$$

The new term $\delta_5^{(4)}$ is a current that integrates to 1 in the direction transverse to a single 5-brane whose class is denoted by $[W]$. The class $[W]$ is the Poincaré dual of an integer sum of all these sources and thus $[W]$ should be an integral class, representing a class in $H_2(X, \mathbb{Z})$. $[W]$ can be further specified taking into account that supersymmetry requires that 5-branes are wrapped on holomorphic curves and thus $[W]$ must correspond to the homology class of holomorphic curves. This fact constrains $[W]$ to be an algebraic class. Further, algebraic classes include negative classes; however, these lead to negative magnetic charges, which are unphysical, and so they have to be excluded. This constrains $[W]$ to be an effective class. Thus, for a given Calabi–Yau 3-fold X the effectivity of $[W]$ constrains the choice of vector bundles V .

The study of the correspondence between the heterotic string (on an elliptic Calabi–Yau 3-fold) and F -theory (on an elliptic Calabi–Yau fourfold) has led Friedman, Morgan, and Witten to introduce a new class of vector bundles which satisfy the anomaly constraint with $[W]$ nonzero. As a result, they prove that the number obtained by integration of $[W]$ over the elliptic fibers of the Calabi–Yau 3-fold agrees with the number of 3-branes given by the Euler characteristic of the Calabi–Yau fourfold divided by 24.

Fourier–Mukai Transforms and Spectral Covers

Let us now describe how the construction of vector bundles out of spectral data (first considered in Hitchin and Beauville, Narasimhan, and Ramanan) can be easily described in the case of elliptic fibrations by means of the relative Fourier–Mukai transform. This construction was widely exploited by Friedman, Morgan, and Witten to construct stable vector bundles on elliptic Calabi–Yau threefolds X , which we will summarize now.

If $V \rightarrow X$ is a vector bundle of rank n which is semistable and of degree 0 on each fibre \mathfrak{f} of $X \rightarrow B$, then its Fourier–Mukai transform $\Phi^1(V)$ is a torsion sheaf of pure dimension 2 on X . The support of $\Phi^1(V)$ is a surface $i: C \hookrightarrow X$, which is finite of degree n over B . Moreover, $\Phi^1(V)$ is of rank 1 on C and, if C is smooth, then $\Phi^1(V) = i_* L$ is just the extension by zero of some line bundle $L \in \text{Pic}(C)$. Conversely, given a sheaf $\mathcal{G} \rightarrow X$ of pure dimension 2 which is flat over B , then $\Phi(\mathcal{G})$ is a vector bundle on X of rank equal to the degree of $\text{supp}(\mathcal{G})$ over B .

This correspondence between vector bundles on X and sheaves on X supported on finite covers of B is known as the spectral cover construction. The torsion sheaf \mathcal{G} is called the spectral sheaf (or line bundle) and the surface $C = \text{supp}(\mathcal{G})$ is called the spectral cover.

For the description of vector bundles on elliptic Calabi–Yau 3-folds X it is appropriate to take $i_* L$ with Chern characters given by $(\eta_E, \eta \in H^2(B, \mathbb{Q}))$ and $a_E, s_E \in \mathbb{Z}$)

$$\text{ch}_0(i_* L) = 0, \quad \text{ch}_1(i_* L) = n\sigma + \pi^* \eta$$

$$\text{ch}_2(i_* L) = \sigma \pi^* \eta_E + a_E \mathfrak{f}, \quad \text{ch}_3(i_* L) = s_E$$

The characteristic classes of the rank- n vector bundle V can be obtained if we apply the Grothendieck–Riemann–Roch theorem to the projection π :

$$\text{ch}(V) = \pi_* [\hat{\pi}^* (\text{ch}(i_* L)) \text{ch}(\mathcal{P}) \text{Td}(T_{X/B})]$$

where $\text{Td}(T_{X/B})$ as given above.

To make sure that the construction leads to $SU(n)$ vector bundles we set $\eta_E = (1/2)nc_1$ giving $c_1(V) = 0$ and the remaining Chern classes are given by

$$c_2(V) = \pi^*(\eta)\sigma + \pi^*(\varpi), \quad c_3(V) = -2\gamma|_S$$

where

$$\varpi = \frac{1}{24}c_1(B)^2(n^3 - n) + \frac{1}{2}(\lambda^2 - \frac{1}{4})n\eta(\eta - nc_1(B))$$

and $\gamma \in H^{1,1}(C, \mathbb{Z})$ is some cohomology class satisfying $\pi_{C*}\gamma = 0 \in H^{1,1}(B, \mathbb{Z})$. The general solution for γ has been derived by Friedman, Morgan, and Witten and is given by $\gamma = \lambda(n\sigma|_C - \pi_C^*\eta + n\pi_C^*c_1(B))$ and $\gamma|_S = -\lambda\pi^*\eta(\pi^*\eta - n\pi^*c_1(B))\sigma$ with $S = C \cap \sigma$. The parameter λ has to be determined such that $c_1(L)$ is an integer class. If n is even, $\lambda = m(m \in \mathbb{Z})$ and in addition we must impose $\eta = c_1(B)$ modulo 2. If n is odd, $\lambda = m + 1/2$.

It remains to discuss the stability of V . The stability depends on the properties of the defining data C and L . If C is irreducible and L a line bundle over C then V will be a vector bundle stable with respect to the polarization

$$J = \epsilon J_0 + \pi^*H_B, \quad \epsilon > 0$$

if ϵ is sufficiently small. This has been proved by Friedman, Morgan, and Witten under the additional assumption that the restriction of V to the generic fiber is regular and semistable. Here J_0 refers to some arbitrary Kähler class on X and H_B a Kähler class on the base B . It implies that the bundle V can be taken to be stable with respect to J while keeping the volume of the fiber \tilde{f} of X arbitrarily small compared to the volumes of effective curves associated with the base. That J is actually a good polarization can be seen by assuming $\epsilon = 0$. Now we observe that π^*H_B is not a Kähler class on X since its integral is non-negative on each effective curve C in X ; however, there is one curve, the fiber \tilde{f} , where the integral vanishes. This means that π^*H_B is on the boundary of the Kähler cone and, to make V stable, we have to move slightly into the interior of the Kähler cone, that is, into the chamber which is closest to the boundary point π^*H_B . Also we note that although π^*H_B is in the boundary of the Kähler cone, we can still define the slope $\mu_{\pi^*H_B}(V)$ with respect to it. Since $(\pi^*H_B)^2$ is some positive multiple of the class of the fiber \tilde{f} , semistability with respect to π^*H_B is implied by the semistability of the restrictions $V|_{\tilde{f}}$ to the fibers. Assume that V is not stable with respect to J , then there is a destabilizing sub-bundle $V' \subset V$ with $\mu_J(V') \geq \mu_J(V)$. But semistability along the fibers says that $\mu_{\pi^*H_B}(V') \leq \mu_{\pi^*H_B}(V)$. If we had equality, it would follow that V' arises by the spectral construction from a proper

subvariety of the spectral cover of V , contradicting the assumption that this cover is irreducible. So we must have a strict inequality $\mu_{\pi^*H_B}(V') < \mu_{\pi^*H_B}(V)$. Now taking ϵ small enough, we can ensure that $\mu_J(V') < \mu_J(V)$, thus V' cannot destabilize V .

D-Branes and Homological Mirror Symmetry

Kontsevich proposed a homological mirror symmetry for a pair (X, Y) of mirror dual Calabi–Yau manifolds; it is conjectured that there exists a categorical equivalence between the bounded derived category $D(X)$ and Fukaya’s A_∞ category $\mathcal{F}(Y)$, which is defined by using the symplectic structure on Y . A Lagrangian submanifold with a flat bundle gives an object of $\mathcal{F}(Y)$. If we consider a locally trivial family of symplectic manifolds Y (i.e., the symplectic form is locally constant as we vary Y in the family) the object of $\mathcal{F}(Y)$ undergoes monodromy transformations going round a loop in the base. On the other hand, the object of $D(X)$ is a complex of coherent sheaves on X and under the categorical equivalence between $D(X)$ and $\mathcal{F}(Y)$ the monodromy (of 3-cycles) is mapped to certain self-equivalences in $D(X)$.

Since all elements in $D(X)$ can be represented by suitable complexes of vector bundles on X , we can consider the topological K -group and the image $K_{\text{hol}}(X)$ of $D(X)$. The Fourier–Mukai transform $\Phi^\epsilon: D(X) \rightarrow D(X)$ induces then a corresponding automorphism $K_{\text{hol}}(X) \rightarrow K_{\text{hol}}(X)$ and also an automorphism on $H^{\text{even}}(X, \mathbb{Q})$ if we use the Chern character ring homomorphism $\text{ch}: K(X) \rightarrow H^{\text{even}}(X, \mathbb{Q})$, as described above. With this in mind, we can introduce various kernels and their associated monodromy transformations.

For instance, let D be the associated divisor defining the large-radius limit in the Kähler moduli space and consider the kernel $\mathcal{O}_\Delta(D)$, with Δ being the diagonal in $X \times X$. The corresponding Fourier–Mukai transform acts on an object $G \in D(X)$ as twisting by a line bundle, that is, $G \mapsto G \otimes \mathcal{O}(D)$. This automorphism is then identified with the monodromy about the large complex structure limit point (LCSL point) in the complex structure moduli space.

Furthermore, if we consider the kernel given by the ideal sheaf \mathcal{I}_Δ on Δ , we find that the action of $\Phi^{\mathcal{I}_\Delta}$ on $H^{\text{even}}(X)$ can be expressed by taking the Chern character ring homomorphism:

$$\begin{aligned} \text{ch}(\Phi^{\mathcal{I}_\Delta}(G)) &= \text{ch}_0(\Phi^{\mathcal{O}_{X \times X}}(G)) - \text{ch}(G) \\ &= \left(\int \text{ch}(G) \cdot \text{Td}(X) \right) - \text{ch}(G) \end{aligned}$$

Kontsevich proposed that this automorphism should reproduce the monodromy about the principal component of the discriminant of the mirror family Y . At the principal component we have vanishing S^3 cycles (and the conifold singularity), thus the action of this monodromy on cohomology may be identified with the Picard–Lefschetz formula.

Now for a given pair of mirror dual Calabi–Yau 3-folds, it is generally assumed that A -type and B -type D-branes exchange under mirror symmetry. For such a pair, Kontsevich’s correspondence between automorphisms of $D(X)$ and monodromies of 3-cycles can then be tested. More specifically, a comparison relies on the identification of two central charges associated to D-brane configurations on both sides of the mirror pair.

For this, we first have to specify a basis for the 3-cycles $\Sigma_i \in H^3(Y, \mathbb{Z})$ such that the intersection form takes the canonical form $\Sigma_i \cdot \Sigma_j = \delta_{i, i+b_{2,1}+1} = \eta_{i,j}$ for $i = 0, \dots, b_{2,1}$. It follows that a 3-brane wrapped about the cycle $\Sigma = \sum_i n_i \Sigma^i$ has an (electric, magnetic) charge vector $\mathbf{n} = (n_i)$. The periods of the holomorphic 3-form Ω are then given by

$$\Pi_i = \int_{\Sigma_i} \Omega$$

and can be used to provide projective coordinates on the complex structure moduli space. If we choose a symplectic basis (A_i, B_j) of $H_2(Y, \mathbb{Z})$ then the A_i periods serve as projective coordinates and the B_j periods satisfy the relations $\Pi^j = \eta_{i,j} \partial \mathcal{F} / \partial \Pi^i$, where \mathcal{F} is the prepotential which has, near the large-radius limit, the asymptotic form (as analyzed by Candelas, Klemm, Theisen, Yau, and Hosono, cf. “Further reading”):

$$\mathcal{F} = \frac{1}{6} \sum_{abc} k_{abc} t_a t_b t_c + \frac{1}{2} \sum_{ab} c_{ab} t_a t_b - \sum_a \frac{c_2(X) J_a}{24} t_a + \frac{\zeta(3)}{2(2\pi i)^3} \chi(X) + \text{const.}$$

where $\chi(X)$ is the Euler characteristic of X , c_{ab} are rational constants (with $c_{ab} = c_{ba}$) reflecting an $\text{Sp}(2h^{1,1} + 2)$ ambiguity, and k_{abc} is the classical triple intersection number given by

$$k_{abc} = \int_X J_a \wedge J_b \wedge J_c$$

The periods determine the central charge $Z(\mathbf{n})$ of a 3-brane wrapped about the cycle $\Sigma = \sum_i n_i [\Sigma_i]$:

$$Z(\mathbf{n}) = \int_{\Sigma} \Omega = \sum_i n_i \Pi_i$$

On the other hand, the central charge associated with an object E of $D(X)$ is given by

$$Z(E) = - \int_X e^{-t_a J_a} \text{ch}(E) \left(1 + \frac{c_2(X)}{24} \right)$$

Now, physically it is assumed that the two central charges are to be identified under mirror symmetry. If we compare the two central charges $Z(\mathbf{n})$ and $Z(E)$, then we obtain a map relating the Chern characters $\text{ch}(E)$ of E to the D-brane charges \mathbf{n} . If we insert the expressions for $\text{ch}(E)$ in $\text{ch}(\Phi^{\mathcal{T}_\Delta}(E))$, it yields a linear transformation acting on \mathbf{n} , such that $n_6 \rightarrow n_6 + n_3$, which agrees with the monodromy transformation about the conifold locus.

Similarly, the monodromy transformation about the LCSL point corresponding to automorphisms $[E] \rightarrow [E \otimes \mathcal{O}_X(D)]$ can be made explicit.

Using the central charge identification, the automorphism/monodromy correspondence has been made explicit for various dual pairs of mirror Calabi–Yau 3-folds (given as hypersurfaces in weighted projective spaces). This identification provides evidence for Kontsevich’s proposal of homological mirror symmetry.

See also: Derived Categories; Mirror Symmetry: A Geometric Survey.

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Four-Manifold Invariants and Physics

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Introduction

Manifolds of dimension 4 play a distinguished role in physics and have done so ever since special and general relativity ushered in the celebrated four-dimensional spacetime. It is also the case that manifolds of dimension 4 play a distinguished role in mathematics: many generalities about manifolds of a general dimension do not apply in dimension 4; there are also phenomena in dimension 4 with no counterpart in other dimensions.

This article describes some of the more important physical and mathematical properties of dimension 4. We begin with an account of some topological and geometric properties for manifolds in general, but avoiding dimension 4, and then embark on the dimension 4 discussion. The references at the end will serve to take the reader further into the subject.

Topological, Piecewise-Linear, and Differentiable Structures for Manifolds

In dealing with topological spaces which are manifolds, one distinguishes three types of manifolds M : topological, piecewise-linear, and differentiable (also called smooth). It is possible to describe the more important differences between these three types using topological techniques.

Consider then a manifold M of dimension n ; M will always be assumed to be compact, connected and

closed unless we indicate the contrary. The type of M is determined by examining whether the transition functions $g_{\alpha\beta}$ are homeomorphisms, (invertible) piecewise-linear maps, or diffeomorphisms. Now, since the transition functions are maps from one subset of \mathbf{R}^n to another, we introduce the groups TOP_n , PL_n , and $DIFF_n$ which are all the homeomorphisms, piecewise-linear maps, and diffeomorphisms of \mathbf{R}^n , respectively. We are naturally led to the three sets of inclusions:

$$\begin{array}{ccccccc} TOP_1 & \subset & TOP_2 & \subset & \cdots & \subset & TOP_n & \subset & \cdots \\ PL_1 & \subset & PL_2 & \subset & \cdots & \subset & PL_n & \subset & \cdots \\ DIFF_1 & \subset & DIFF_2 & \subset & \cdots & \subset & DIFF_n & \subset & \cdots \end{array} \quad [1]$$

For each of the three sets of inclusions we pass to the direct limit and construct the three limiting groups

$$TOP, \quad PL, \quad DIFF \quad [2]$$

With these three groups are associated the classifying spaces $BTOP$, BPL and $BDIFF$. The transition functions $g_{\alpha\beta}$ are those of the tangent bundle to M ; and there are three possible tangent bundles depending on the type of M and we denote these tangent bundles by TM_{TOP} , TM_{PL} , and TM_{DIFF} in an obvious notation. Then to determine the tangent bundles TM_{TOP} , TM_{PL} , and TM_{DIFF} one simply selects an element of the homotopy classes

$$[M, BTOP], \quad [M, BPL], \quad \text{and} \quad [M, BDIFF] \quad [3]$$

respectively.

Given this threefold hierarchy of manifold structures one wishes to know when one can straighten out a topological manifold to make it piecewise linear; and also, when can one *smooth* a piecewise-linear manifold to make it differentiable?

If $\dim M \geq 5$ of M these two questions can be formulated as lifting problems.

TOP versus PL for $\dim M \neq 4$

Taking the first of them, so that we are comparing piecewise-linear and topological structures on M , one can check BPL fibers over $BTOP$ with fiber TOP/PL yielding

$$\begin{array}{ccc} TOP/PL & \rightarrow & BPL \\ & \downarrow \pi & \\ & BTOP & \end{array} \quad [4]$$

A method for *straightening out* a PL manifold is now apparent: now a topological manifold is a choice of map $\alpha: M \rightarrow BTOP$, and a *factorization* of α through BPL will give M a PL structure. We show this below

$$\begin{array}{ccc} & BPL & \\ \beta \nearrow & \downarrow \pi & \alpha = \pi \circ \beta \\ M & \xrightarrow{\alpha} & BTOP \end{array} \quad [5]$$

The existence of the map $\beta: M \rightarrow BPL$ satisfying $\alpha = \pi \circ \beta$ provides M with a PL structure and is a *lifting* of the map α from the base $BTOP$ to the total space BPL .

This lifting method, for passing from TOP structures to PL structures, does work, *provided* $\dim M \geq 5$, since we have the stability result that

$$\frac{TOP_n}{PL_n} \simeq \frac{TOP}{PL}, \quad n \geq 5 \quad [6]$$

For the map β to exist the obstructions to the lifting which are cohomology classes of the form

$$H^{k+1}(M; \pi_k(TOP/PL)) \quad [7]$$

must vanish. However, Kirby and Siebenmann have shown that

$$TOP/PL \simeq K(Z_2, 3) \quad [8]$$

where $K(Z_2, 3)$ is *Eilenberg–Mac Lane space* so that its sole nonvanishing homotopy group is in dimension 3 giving us

$$\pi_n(TOP/PL) = \begin{cases} Z_2 & \text{if } n = 3 \\ 0 & \text{otherwise} \end{cases} \quad [9]$$

Any obstruction to β 's existence is a class $e(M)$, say, in

$$H^4(M; Z_2) \quad \dim M \geq 5 \quad [10]$$

When $e(M)$ *vanishes*, the map β exists and furnishes M with a PL structure; if $e(M) \neq 0$ it is natural to go on to ask how many (homotopy classes of) such β 's exist? Standard obstruction theory says the relevant

homotopy classes are just the whole cohomology group

$$H^k(M; \pi_k(TOP/PL)) \quad [11]$$

which, since $k = 3$, is just

$$H^3(M; Z_2) \quad [12]$$

So, for $\dim M \geq 5$, we see that when a closed topological manifold M acquires a PL structure by the lifting process just described, then the possible distinct PL structures are isomorphic to

$$H^3(M; Z_2) \quad [13]$$

which is not zero in general.

Finally, if $\dim M \leq 3$, then the notions PL and TOP coincide, so we are left with the case $\dim M = 4$ which we shall come to below. Now we wish to describe the next step in the sequence TOP, PL, DIFF which is the smoothing problem.

PL versus DIFF for $\dim M \neq 4$

Similar ideas are used to address the question of smoothing a piecewise-linear manifold – however, the results are different. Let us assume that M is a closed PL manifold with $\dim M \geq 5$. This time the fibration is

$$\begin{array}{ccc} PL/DIFF & \rightarrow & BDIFF \\ & \downarrow \pi & \\ & BPL & \end{array} \quad [14]$$

The smoothing of a piecewise-linear M can also be handled with obstruction theory and leads us immediately to the consideration of the homotopy groups $\pi_n(PL/DIFF)$. This time the nontrivial homotopy groups of the fiber are much more numerous than in the piecewise-linear case. In fact one has

$$\pi_n(PL/DIFF) = \begin{cases} 0 & \text{if } n \leq 6 \\ Z_{28} & \text{if } n = 7 \\ Z_2 & \text{if } n = 8 \\ \vdots & \vdots \\ Z_{992} & \text{if } n = 11 \\ \vdots & \vdots \end{cases} \quad [15]$$

The obstructions to passing from a PL to a DIFF structure on M now lie in

$$H^{k+1}(M; \pi_k(PL/DIFF)) \quad [16]$$

and the number of distinct liftings comprises the cohomology group

$$H^k(M; \pi_k(PL/DIFF)) \quad [17]$$

As an illustration of all this, consider the case $M = S^7$; then the first nontriviality occurs when $n = 7$ and so the obstruction to smoothing S^7 lies in

$$H^8(S^7; \pi_7(PL/DIFF)) \quad [18]$$

which is of course zero – this means that S^7 can be smoothed, a fact which we know from first principles. However, by the obstruction theory introduced above, the resulting smooth structures are isomorphic to

$$H^7(S^7; \pi_7(PL/DIFF)) = H^7(S^7; \mathbb{Z}_{28}) = \mathbb{Z}_{28} \quad [19]$$

Hence, we have the celebrated result of Milnor and Kervaire and Milnor that S^7 has 28 distinct differentiable structures, 27 of which correspond to what are known as *exotic spheres*.

Lastly, if $\dim M \leq 3$, then PL and DIFF coincide – this leaves us with the case of greatest interest namely $\dim M = 4$.

The Strange Case of Four Dimensions

In four dimensions there are phenomena which have no counterpart in any other dimension. First of all, there are topological 4-manifolds which have no smooth structure, though if they have a PL structure, then they possess a unique smooth structure. Second, the impediment to the existence of a smooth structure is of a completely different type to that met in the standard obstruction theory – it is not the pullback of an element in the cohomology of a classifying space, that is, it is not a characteristic class. Also the four-dimensional story is far from completely known. Nevertheless, there are some very striking results dating from the early 1980s onwards.

We begin by disposing of the difference between PL and DIFF structures: our earlier results together with the vanishing statement

$$\pi_n(PL/DIFF) = 0, \quad n \leq 6 \quad [20]$$

mean that every PL 4-manifold possesses a unique DIFF structure. Thus, we can take the crucial difference to be between DIFF and TOP.

In Freedman (1982) all, simply connected, *topological* 4-manifolds were classified by their intersection form q .

We recall that q is a quadratic form constructed from the cohomology of M as follows: take two elements α and β of $H^2(M; \mathbb{Z})$ and form their cup product $\alpha \cup \beta \in H^4(M; \mathbb{Z})$; then we define $q(\alpha, \beta)$ by

$$q(\alpha, \beta) = (\alpha \cup \beta)[M] \quad [21]$$

where $(\alpha \cup \beta)[M]$ denotes the integer obtained by evaluating $\alpha \cup \beta$ on the generating cycle $[M]$ of the

top homology group $H_4(M; \mathbb{Z})$ of M . Poincaré duality ensures that such a form is always non-degenerate over \mathbb{Z} and so has $\det q = \pm 1$; q is then called unimodular. Also we refer to q , as “even” if all its diagonal entries are even, and as “odd” otherwise.

Freedman’s work yields the following:

Theorem (Freedman). *A simply connected 4-manifold M with even intersection form q belongs to a unique homeomorphism class, while if q is odd there are precisely two nonhomeomorphic manifolds M with q as their intersection form.*

This is a very powerful result – the intersection form q very nearly determines the homeomorphism class of a simply connected M , and actually only fails to do so in the odd case where there are still just two possibilities. Further, *every* unimodular quadratic form occurs as the intersection form of some manifold.

As an illustration of the impressive nature of Freedman’s work, choose M to be the sphere S^4 , since $H^2(S^4; \mathbb{Z})$ is trivial, then q is the zero quadratic form and is of course even; we write this as $q = \emptyset$. Now recollect that the *Poincaré conjecture* in four dimensions is the statement that any homotopy 4-sphere, S^4_b say, is actually *homeomorphic* to S^4 . Well, since $H^2(S^4_b; \mathbb{Z})$ is also trivial then any S^4_b also has intersection form $q = \emptyset$. Applying Freedman’s theorem to S^4_b immediately asserts that S^4_b belongs to a unique homeomorphism class which must be that of S^4 thereby establishing the Poincaré conjecture.

Freedman’s result combined with a much earlier result of Rohlin (1952) also gives us an example of a nonsmoothable 4-manifold: Rohlin’s theorem asserts that given a smooth, simply connected, 4-manifold with even intersection form q , then the signature – the signature of q being defined to be the difference between the number of positive and negative eigenvalues of $q - \sigma(q)$ of q is divisible by 16.

Now write

$$q = \begin{pmatrix} 2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 2 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 2 \end{pmatrix} = E_8 \quad [22]$$

(E_8 is actually the Cartan matrix for the exceptional Lie algebra e_8), then, by inspection, q is even, and by calculation, it has signature 8. By Freedman’s theorem there is a single, simply connected, 4-manifold with intersection form $q = E_8$. However, by

Rohlin's theorem, it cannot be smoothed since its signature is 8.

The next breakthrough was due to Donaldson (1983). Donaldson's theorem is applicable to definite forms q , which by appropriate choice of orientation on M we can take to be *positive* definite. One has:

Theorem (Donaldson). *A simply connected, smooth 4-manifold, with positive-definite intersection form q is always diagonalizable over the integers to $q = \text{diag}(1, \dots, 1)$.*

One can immediately deduce that no, simply connected, 4-manifold for which q is even and positive definite can be smoothed!

For example, the manifold with $q = E_8 \oplus E_8$ has signature 16 (by Rohlin's theorem). But since E_8 is even, then so is $E_8 \oplus E_8$ and so Donaldson's theorem forbids such a manifold from existing smoothly.

In fact, in contrast to Freedman's theorem, which allows *all* unimodular quadratic forms to occur as the intersection form of some topological manifold, Donaldson's theorem says that in the positive-definite, smooth, case only *one* quadratic form is allowed, namely I .

Donaldson's work makes contact with physics because it uses the *Yang-Mills equations* as we now outline.

Let A be a connection on a principal $SU(2)$ bundle over a simply connected 4-manifold M with positive-definite intersection form. If the curvature 2-form of A is F , then F has an L^2 norm which is the Euclidean Yang-Mills action S . One has

$$S = \|F\|^2 = - \int_M \text{tr}(F \wedge *F) \quad [23]$$

where $*F$ is the usual dual 2-form to F . The minima of the action S are given by those A , called instantons, which satisfy the famous self-duality equations

$$F = *F \quad [24]$$

Given one instanton A which minimizes S one can perturb about A in an attempt to find more instantons. This process is successful and the space of all instantons can be fitted together to form a global moduli space of finite dimension. For the instanton which provides the absolute minimum of S , the moduli space \mathcal{M} is a noncompact space of dimension 5.

We can now summarize the logic that is used to prove Donaldson's theorem: there are very strong relationships between M and the moduli space \mathcal{M} ;

for example, let q be regarded as an $n \times n$ matrix with precisely p unit eigenvalues (clearly $p \leq n$ and Donaldson's theorem is just the statement that $p = n$), then \mathcal{M} has precisely p singularities which look like cones on the space CP^2 . These combine to produce the result that the 4-manifold M has the same topological signature $\text{Sign}(M)$ as p copies of CP^2 ; and so they have signature $a - b$, where a of the CP^2 's are oriented as usual and b have the opposite orientation. Thus,

$$\text{Sign}(M) = a - b \quad [25]$$

Now by definition, $\text{Sign}(M)$ is the signature $\sigma(q)$ of the intersection form q of M . But, by assumption, q is positive definite $n \times n$ so $\sigma(q) = n = \text{Sign}(M)$. Hence,

$$n = a - b \quad [26]$$

However, $a + b = p$ and $p \leq n$ so we can say that

$$n = a - b, \quad p = a + b \leq n \quad [27]$$

but one always has $a + b \geq a - b$ so we have

$$n \leq p \leq n \Rightarrow p = n \quad [28]$$

which is Donaldson's theorem.

Donaldson's Polynomial Invariants

Donaldson extended his work by introducing polynomial invariants also derived from Yang-Mills theory and to discuss them we must introduce some notation.

Let M be a smooth, simply connected, orientable Riemannian 4-manifold without boundary and A be an $SU(2)$ connection which is anti-self-dual so that

$$F = - * F \quad [29]$$

Then the space of all gauge-inequivalent solutions to this anti-self-duality equation – the moduli space \mathcal{M}_k – has a dimension given by the integer

$$\dim \mathcal{M}_k = 8k - 3(1 + b_2^+) \quad [30]$$

Here k is the instanton number which gives the topological type of the solution A . The instanton number is minus the second Chern class $c_2(F) \in H^2(M; \mathbb{Z})$ of the bundle on which the A is defined. This means that we have

$$k = -c_2(F)[M] = \frac{1}{8\pi^2} \int_M \text{tr}(F \wedge F) \in \mathbb{Z} \quad [31]$$

The number b_2^+ is defined to be the rank of the positive part of the intersection form q of M .

A Donaldson invariant $q_{d,r}^M$ is a symmetric integer polynomial of degree d in the 2-homology $H_2(M; \mathbb{Z})$ of M

$$q_{d,r}^M : \underbrace{H_2(M) \times \cdots \times H_2(M)}_{d \text{ factors}} \longrightarrow \mathbb{Z} \quad [32]$$

Given a certain map m_i ,

$$m_i : H_i(M) \rightarrow H^{4-i}(\mathcal{M}_k) \quad [33]$$

if $\alpha \in H_2(M)$ and $*$ represents a point in M , we define $q_{d,r}^M(\alpha)$ by writing

$$q_{d,r}^M(\alpha) = m_2^d(\alpha) m_0^r(*) [\mathcal{M}_k] \quad [34]$$

The evaluation of $[\mathcal{M}_k]$ on the RHS of the above equation means that

$$2d + 4r = \dim \mathcal{M}_k \quad [35]$$

so that \mathcal{M}_k is even dimensional; this is achieved by requiring b_2^+ to be odd.

Now the Donaldson invariants $q_{d,r}^M$ are *differential* topological invariants rather than topological invariants but they are difficult to calculate as they require detailed knowledge of the instanton moduli space \mathcal{M}_k . However they are nontrivial and their values are known for a number of 4-manifolds M . For example, if M is a complex algebraic surface, a positivity argument shows that they are nonzero when d is large enough. Conversely, if M can be written as the connected sum

$$M = M_1 \# M_2$$

where both M_1 and M_2 have $b_2^+ > 0$, then they all vanish.

Topological Quantum Field Theories

Turning now to physics, it is time to point out that the $q_{d,r}^M$ can also be obtained, Witten (1988), as the correlation functions of twisted $N=2$ supersymmetric topological quantum field theory.

The action S for this theory is given by

$$\begin{aligned} S = \int_M d^4x \sqrt{g} \operatorname{tr} \left\{ \frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \frac{1}{4} F_{\mu\nu}^* F^{\mu\nu} \right. \\ \left. + \frac{1}{2} \phi D_\mu D^\mu \lambda + i D_\mu \psi_\nu \chi^{\mu\nu} - i \eta D_\mu \psi^\mu \right. \\ \left. - \frac{i}{8} \phi [\chi_{\mu\nu}, \chi^{\mu\nu}] - \frac{i}{2} \lambda [\psi_\mu, \psi^\mu] \right. \\ \left. - \frac{i}{2} \phi [\eta, \eta] - \frac{1}{8} [\phi, \lambda]^2 \right\} \quad [36] \end{aligned}$$

where $F_{\mu\nu}$ is the curvature of a connection A_μ and $(\phi, \lambda, \eta, \psi_\mu, \chi_{\mu\nu})$ are a collection of fields introduced

in order to construct the right supersymmetric theory; ϕ and λ are both spinless while the multiplet $(\psi_\mu, \chi_{\mu\nu})$ contains the components of a 0-form, a 1-form, and a self-dual 2-form, respectively.

The significance of this choice of multiplet is that the instanton deformation complex used to calculate $\dim \mathcal{M}_k$ contains precisely these fields.

Even though S contains a metric, its correlation functions are *independent* of the metric g so that S can still be regarded as a topological quantum field theory. This is because both S and its associated energy momentum tensor $T \equiv (\delta S / \delta g)$ can be written as BRST commutators $S = \{Q, V\}, T = \{Q, V'\}$ for suitable V and V' .

With this theory, it is possible to show that the correlation functions are *independent* of the gauge coupling and hence we can evaluate them in a small coupling limit. In this limit, the functional integrals are dominated by the classical minima of S , which for A_μ are just the instantons

$$F_{\mu\nu} = -F_{\mu\nu}^* \quad [37]$$

We also need ϕ and λ to vanish for irreducible connections. If we expand all the fields around the minima up to quadratic terms and do the resulting Gaussian integrals, the correlation functions may be formally evaluated.

A general correlation function of this theory is given by

$$\langle P \rangle = \int \mathcal{D}\mathcal{F} \exp[-S] P(\mathcal{F}) \quad [38]$$

where \mathcal{F} denotes the collection of fields present in S and $P(\mathcal{F})$ is some polynomial in the fields.

S has been constructed so that the zero modes in the expansion about the minima are the tangents to the moduli space \mathcal{M}_k . This suggests doing the $\mathcal{D}\mathcal{F}$ integration as follows: express the integral as an integral over modes, then integrate out all the nonzero modes first leaving a *finite-dimensional* integration over the compactified moduli space $\overline{\mathcal{M}}_k$. The Gaussian integration over the nonzero modes is a boson-fermion ratio of determinants, which supersymmetry constrains to be ± 1 , bosonic and fermionic eigenvalues being equal in pairs.

This amounts to writing

$$\langle P \rangle = \int_{\overline{\mathcal{M}}_k} P_n \quad [39]$$

where P_n denotes some n -form over $\overline{\mathcal{M}}_k$ and $n = \dim \overline{\mathcal{M}}_k$. If the original polynomial $P(\mathcal{F})$ is judiciously chosen, then calculation of $\langle P \rangle$ reproduces evaluation of the Donaldson polynomials $q_{d,r}^M$.

The Seiberg–Witten Equations

The Seiberg–Witten equations constitute another breakthrough in the work on the topology of 4-manifolds, since they greatly simplify the calculation of the data supplied by the Donaldson polynomial invariants. We shall discuss this later below but turn now to the equations themselves.

If we choose an oriented, compact, closed, Riemannian manifold M , then the data we need for the Seiberg–Witten equations are a connection A on a line bundle L over M and a “local spinor” field ψ . The Seiberg–Witten equations are then

$$\not{D}_A \psi = 0, \quad F^+ = -\frac{1}{2} \bar{\psi} \Gamma \psi \quad [40]$$

where \not{D}_A is the Dirac operator and Γ is made from the gamma matrices Γ_i according to $\Gamma = (1/2)[\Gamma_i, \Gamma_j] dx^i \wedge dx^j$.

We call ψ a local spinor because global spinors may not exist on M ; however, in dimension 4, orientability guarantees that a spin_c structure exists on M (a choice of spin_c structure on M is an extra piece of data in the Seiberg–Witten case); ψ is then the appropriate section for the spin_c bundle and behaves locally like a spinor coupled to the $U(1)$ connection A . Let $\text{Spin}_c(M)$ denote the set of isomorphism classes of spin_c structures on M then, for the case $b_2^+ > 1$ – the case $b_2^+ = 1$ has some technicalities – the Seiberg–Witten invariants determine a map SW of the form

$$\text{SW} : \text{Spin}_c(M) \longrightarrow \mathbb{Z} \quad [41]$$

We emphasize that A is just a $U(1)$ abelian connection and so $F = dA$, with F^+ denoting the self-dual part of F .

We shall now have a look at an example of a new result obtained directly from the Seiberg–Witten equations. The equations clearly provide the absolute minima for the action

$$S = \int_M \left\{ |\not{D}_A \psi|^2 + \frac{1}{2} |F^+|^2 + \frac{1}{2} \bar{\psi} \Gamma \psi \right\} \quad [42]$$

If we use a Weitzenböck formula to relate the Laplacian $\nabla_A^* \nabla_A$ to $\not{D}_A^* \not{D}_A$ plus curvature terms, we find that S satisfies

$$\begin{aligned} & \int_M \left\{ |\not{D}_A \psi|^2 + \frac{1}{2} |F^+|^2 + \frac{1}{2} \bar{\psi} \Gamma \psi \right\} \\ &= \int_M \left\{ |\nabla_A \psi|^2 + \frac{1}{2} |F^+|^2 + \frac{1}{8} |\psi|^4 + \frac{1}{4} R |\psi|^2 \right\} \quad [43] \end{aligned}$$

$$\begin{aligned} &= \int_M \left\{ |\nabla_A \psi|^2 + \frac{1}{4} |F|^2 + \frac{1}{8} |\psi|^4 + \frac{1}{4} R |\psi|^2 \right\} \\ &+ \pi^2 c_1^2(L) \quad [44] \end{aligned}$$

where R is the scalar curvature of M and $c_1(L)$ is the Chern class of L .

We notice that the action now looks like one for monopoles. But now suppose that R is positive and that the pair (A, ψ) is a solution to the Seiberg–Witten equations, then the left-hand side (LHS) of this last expression is zero and all the integrands on the RHS are positive so the solution must obey $\psi = 0$ and $F^+ = 0$. A technical point is that if M has $b_2^+ > 1$, then a perturbation of the metric can preserve the positivity of R but perturb $F^+ = 0$ to be simply $F = 0$ rendering the connection A flat. Hence, in these circumstances, the solution (A, ψ) is the trivial one. This means that we have a new kind of vanishing theorem in four dimensions.

Theorem (Witten 1994). *No 4-manifold with $b_2^+ > 1$ and nontrivial solution to the Seiberg–Witten equations admits a metric of positive scalar curvature.*

Now, for technical reasons, we assume that the $q_{d,r}^M$ have the property that

$$q_{d,r+2}^M = 4q_{d,r}^M \quad [45]$$

A simply connected M with this property is called of *simple type*. We also define \tilde{q}_d^M by writing

$$\tilde{q}_d^M = \begin{cases} q_{d,0}^M, & \text{if } d = (b_2^+ + 1) \bmod 2 \\ \frac{1}{2} q_{d,1}^M, & \text{if } d = b_2^+ \bmod 2 \end{cases} \quad [46]$$

The generating function $G_M(\alpha)$ is now given by

$$G_M(\alpha) = \sum_{d=0}^{\infty} \frac{1}{d!} \tilde{q}_d^M(\alpha) \quad [47]$$

According to Kronheimer and Mrowka (1994), $G_M(\alpha)$ can be expressed in terms of a *finite* number of classes (known as *basic classes*) κ_i ($\kappa_i \in H^2(M)$) with rational coefficients a_i (the Seiberg–Witten invariants) resulting in the formula

$$G_M(\alpha) = \exp[\alpha \cdot \alpha / 2] \sum_i a_i \exp[\kappa_i \cdot \alpha] \quad [48]$$

Hence, for M of simple type, the polynomial invariants are determined by a (finite) number of basic classes and the Seiberg–Witten invariants.

Returning now to the physics we find that the quantum field theory approach to the polynomial invariants relates them to properties of the moduli space for the Seiberg–Witten equations rather than to properties of the instanton moduli space \mathcal{M}_k .

The moduli space for the Seiberg–Witten equations, unlike the instanton case, is *compact* and generically has dimension

$$\frac{c_1^2(L) - 2\chi(M) - 3\sigma(M)}{4} \quad [49]$$

$\chi(M)$ and $\sigma(M)$ being the Euler characteristic and signature of M , respectively. When

$$c_1^2(L) = 2\chi(M) + 3\sigma(M) \quad [50]$$

we get a zero-dimensional moduli space consisting of a finite collection of points

$$\{P_1, \dots, P_N\} \quad [51]$$

Now each point P_i has a sign $\epsilon_i = \mp 1$ associated with it coming from the sign of the determinant of elliptic operator whose index gave the dimension of the moduli space. The sum of these signs is an integer topological invariant denoted by n_L , that is,

$$n_L = \sum_{i=1}^N \epsilon_i \quad [52]$$

Returning now to our formula for $G_M(\alpha)$, one finds that

$$G_M(\alpha) = 2^{b(M)} \exp[\alpha \cdot \alpha / 2] \sum_T n_L \exp[c_1(L) \cdot \alpha] \quad [53]$$

$$p(M) = 1 + \frac{1}{4}(7\chi(M) + 11\sigma(M)) \quad [54]$$

and the sum over L on the RHS of the formula is over line bundles L that satisfy

$$c_1^2(L) = 2\chi(M) + 3\sigma(M) \quad [55]$$

that is, it is a sum over L with zero-dimensional Seiberg–Witten moduli spaces.

Comparison of the two formulas for $G_M(\alpha)$ – the first mathematical in origin and the second physical – allows one to identify the Seiberg–Witten invariants a_i and the Kronheimer–Mrowka basic classes κ_i as the $c_1(L)$'s.

The results described thus far are for *simply connected* 4-manifolds but this condition is not obligatory for and there is also a theory in the non-simply-connected case (Mariño and Moore 1999).

The physics underlying these topological results is of great importance since many of the ideas originate there. It is known that the computation of the Donaldson invariants there uses the fact that the $N=2$ gauge theory is asymptotically free. This means that the ultraviolet limit being one of weak coupling is tractable. However, the less tractable infrared or strong-coupling limit would do just as well to calculate the Donaldson invariants since these latter are metric independent.

In Seiberg and Witten's work, this infrared behavior is actually determined and it is found that, in the strong-coupling infrared limit, the theory is equivalent to a *weakly coupled* theory of abelian fields and monopoles. There is also a duality

between the original theory and the theory with monopoles which is expressed by the fact that the (abelian) gauge group of the monopole theory is the dual of the maximal torus of the group of the nonabelian theory.

We recall that the Yang–Mills gauge group in this discussion is $SU(2)$. Seiberg and Witten's results mean the replacement of $SU(2)$ instantons used to compute the Donaldson invariants by the counting of $U(1)$ monopoles. This calculation of the non-abelian Donaldson data by abelian Seiberg–Witten data theory is much like the representation theory of a nonabelian Lie group G where everything is determined by an abelian object: the maximal torus.

The theory considered by Seiberg and Witten possesses a collection of quantum vacua labeled by a complex parameter u which turns out to parametrize a family of elliptic curves. A central part is played by a function $\tau(u)$ on which there is a modular action of $SL(2, \mathbb{Z})$. The successful determination of the infrared limit involves an electric–magnetic duality and the whole matter is of very considerable independent interest for quantum field theory, quark confinement, and string theory in general.

Seiberg–Witten Theory and Exotic Structures on 4-Manifolds

We saw earlier that, when $\dim M \neq 4$, a manifold may possess a finite number of differentiable structures, S^7 having 28 distinct smooth structures. However, in dimension 4, Seiberg–Witten theory has been used to show that there are many 4-manifolds with a countable infinity of smooth structures. We just mention two: the $K3$ surface has infinitely many smooth structures as does the manifold $\mathbb{C}P^2 \# 5\overline{\mathbb{C}P^2}$. This is another instance of how dimension 4 differs from all other dimensions. This infinite variety of exotic smooth structures in four dimensions is also of great interest to physics.

An outstanding four-dimensional matter still is the *smooth Poincaré conjecture* which asks whether a smooth 4-manifold M homotopic to S^4 is *diffeomorphic* to S^4 ? Such an M is certainly *homeomorphic* to S^4 because this is the standard Poincaré conjecture proved by Freedman and, if the answer to this question is yes then S^4 would be an example of a 4-manifold with no exotic smooth structures. There is at present no consensus on the answer to this question.

Exotic Structures on Open 4-Manifolds

If M is an open manifold, that is, a noncompact manifold without boundary, and $M = \mathbb{R}^n$ then, for

$n \neq 4$, there is only one smooth structure; but for $n=4$, there are exotic differentiable structures on \mathbb{R}^4 . In fact, Gompf showed that there is a *continuum* of exotic differentiable structures that can be placed on \mathbb{R}^4 .

Symplectic and Kähler 4-Manifolds

Many 4-manifolds are symplectic, and symplectic manifolds are central in physics; there are many results obtained using Seiberg–Witten theory concerning the topology and geometry of symplectic manifolds. The exotic K3 structures referred to above are all symplectic and so there is no shortage of symplectic structures even within one homeomorphism class. Taubes obtained far-reaching new results for symplectic 4-manifolds including establishing an equivalence between the Seiberg–Witten invariants in the symplectic case and the Gromov invariants.

Kähler manifolds possess, simultaneously, compatible, Riemannian, symplectic and complex structures and, beginning with Witten's work, there are many results to be found for Kähler 4-manifolds using Seiberg–Witten techniques.

4-Manifolds with Boundary

There is a very important extension of the Donaldson–Seiberg–Witten theory to 4-manifolds M with boundary $\partial M = N$. When $\partial M \neq \emptyset$, the Donaldson invariants are not numerical invariants but take values in $\text{HF}(N)$ where $\text{HF}(N)$ denotes what is called the Floer homology of the 3-manifold N . Topological quantum field theory is the ideal setting for this theory since it naturally treats manifolds with boundaries. The Floer homology groups $\text{HF}(N)$ act as Hilbert spaces for the quantum fields defined on the boundary. There is now a full interplay of 4-manifold theory and 3-manifold theory as well as Yang–Mills theory in three and four dimensions. This interplay is often realized by taking two 4-manifolds M_1 and M_2 with the same boundary N and joining them along N to obtain a *closed 4-manifold* M so that

$$M = M_1 \cup_N M_2 \quad [56]$$

Given a 3-manifold N , and an $\text{SU}(2)$ connection A , Floer studied the critical points of the Chern–Simons function $f(A)$ defined by

$$f(A) = \frac{1}{8\pi^2} \int_N \text{tr}(A \wedge dA + \frac{2}{3} A \wedge A \wedge A) \quad [57]$$

where $f(A)$ is regarded as a function on the infinite-dimensional space \mathcal{A} of connections. The function $f(A)$ changes by an integer under a gauge transformation and so descends to a single-valued gauge-invariant

function on the space of gauge orbits \mathcal{A}/\mathcal{G} if one considers $\exp(2\pi k i f(A))$ where $k \in \mathbb{Z}$ (\mathcal{G} being the group of gauge transformations). Morse theory applied to this infinite-dimensional setting gives an infinite Morse index to each critical point, a pathology which is avoided by only defining the difference of the index between two critical points using spectral flow. The critical points correspond, via gradient flow and a consideration of the instanton equations

$$F = \pm * F \quad [58]$$

on the 4-manifold $N \times \mathbb{R}$, to the flat connections on the 3-manifold N . The latter are identifiable as the set of (equivalence classes) of representations of the fundamental group $\pi_1(M)$ in the gauge group $\text{SU}(2)$, that is, with

$$\text{Hom}(\pi_1(N), \text{SU}(2))/\text{Ad } \text{SU}(2) \quad [59]$$

For the Seiberg–Witten formulation, let \hat{A} denote a connection on the 3-manifold N with curvature $F(\hat{A})$. Then the Chern–Simons function $f(A)$ is replaced by the abelian Chern–Simons function together with a quadratic fermion term resulting in the function $f^{\text{SW}}(\hat{A})$, defined by

$$f^{\text{SW}}(\hat{A}) = \int_N \left\{ \phi \mathcal{D}_{\hat{A}} \phi + \hat{A} \wedge F(\hat{A}) \right\} \quad [60]$$

where $\mathcal{D}_{\hat{A}}$ denotes the self-adjoint Dirac operator in three dimensions acting on a spinor ϕ on N ; because of the presence of the Chern–Simons function $f^{\text{SW}}(\hat{A})$ is only defined up to a multiple of $8\pi^2$ in a manner similar to the case for $f(A)$. Gradient flow together with the Seiberg–Witten equations on the 4-manifold $N \times \mathbb{R}$ result in critical points corresponding to the solutions to

$$\mathcal{D}_{\hat{A}} \phi = 0, \quad F(\hat{A}) = -\frac{1}{2} \phi \Gamma \phi \quad [61]$$

which is a three-dimensional version of the Seiberg–Witten equations.

The critical point theory of these two functions $f(A)$ and $f^{\text{SW}}(\hat{A})$ permit the construction of the instanton Floer homology groups $\text{HF}^{\text{inst}}(N)$ and $\text{HF}^{\text{SW}}(N)$, respectively. In fact, there are several kinds of Floer homology: Lagrangian Floer homology, instanton Floer homology, Heegard–Floer homology, Seiberg–Witten–Floer homology and conjectures concerning their relations to one another.

There are still many unanswered questions of joint interest to mathematicians and physicists in the entire area of 4-manifold theory.

See also: Electric–Magnetic Duality; Gauge Theoretic Invariants of 4-Manifolds; Floer Homology; Topological Quantum Field Theory: Overview.

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Fractal Dimensions in Dynamics

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Introduction

Since the 1970s, dimension theory for dynamics has evolved into an independent field of mathematics. Its main goal is to measure complexity of invariant sets and measures using fractal dimensions. The history of fractal dimensions is closely related to the names of H Minkowski (Minkowski content, 1903), H Hausdorff (Hausdorff dimension, 1919), G Bouligand (Bouligand dimension, 1928), L S Pontryagin and L G Schnirelmann (metric order, 1932), P Moran (Moran geometric constructions, 1946), A S Besicovitch and S J Taylor (Besicovitch–Taylor index, 1954), A Rényi (Rényi spectrum for dimensions, 1957), A N Kolmogorov and V M Tihomirov (metric dimension, Kolmogorov

complexity, 1959), Ya G Sinai, D Ruelle, R Bowen (thermodynamic formalism, Bowen’s equation, 1972, 1973, 1979), B Mandelbrot (fractals and multifractals, 1974), J L Kaplan and J A Yorke (Lyapunov dimension, 1979), J E Hutchinson (fractals and self-similarity, 1981), C Tricot, D Sullivan (packing dimension, 1982, 1984), H G E Hentschel and I Procaccia (Hentschel–Procaccia spectrum for dimensions, 1983), Ya Pesin (Carathéodory–Pesin dimension, 1988), M Lapidus and M van Frankenhuysen (complex dimensions for fractal strings, 2000), etc. Fractal dimensions enable us to have a better insight into the dynamics appearing in various problems in physics, engineering, chemistry, medicine, geology, meteorology, ecology, economics, computer science, image processing, and, of course, in many branches of mathematics. Concentrating on box and Hausdorff dimensions only, we describe basic methods of fractal analysis in dynamics, sketch their applications, and indicate some trends in this rapidly growing field.

Fractal Dimensions

Box Dimensions

Let A be a bounded set in \mathbb{R}^N , and let $d(x, A)$ be Euclidean distance from x to A . The Minkowski sausage of radius ε around A (a term coined by B Mandelbrot) is defined as ε -neighborhood of A , that is, $A_\varepsilon := \{y \in \mathbb{R}^N : d(y, A) < \varepsilon\}$. By the upper s -dimensional Minkowski content of A , $s \geq 0$, we mean

$$\mathcal{M}^{*s}(A) := \overline{\lim}_{\varepsilon \rightarrow 0} \frac{|A_\varepsilon|}{\varepsilon^{N-s}} \in [0, \infty]$$

Here $|\cdot|$ denotes N -dimensional Lebesgue measure. The corresponding upper box dimension is defined by

$$\overline{\dim}_B A := \inf\{s \geq 0 : \mathcal{M}^{*s}(A) = 0\}$$

The lower s -dimensional Minkowski content $\mathcal{M}_*^s(A)$ and the corresponding lower box dimension $\underline{\dim}_B A$ are defined analogously. The name of box dimension stems from the following: if we have an ε -grid in \mathbb{R}^N composed of closed N -dimensional boxes with side ε , and if $N(A, \varepsilon)$ is the number of boxes of the grid intersecting A , then

$$\overline{\dim}_B A = \overline{\lim}_{\varepsilon \rightarrow 0} \frac{\log N(A, \varepsilon)}{\log(1/\varepsilon)}$$

and analogously for $\underline{\dim}_B A$. It suffices to take any geometric subsequence $\varepsilon_k = b^{-k}$ in the limit, where $b > 1$ (H Furstenberg, 1970). There are many other names for the upper box dimension appearing in the literature, like the Cantor–Minkowski order, Minkowski dimension, Bouligand dimension, Borel logarithmic rarefaction, Besicovitch–Taylor index, entropy dimension, Kolmogorov dimension, fractal dimension, capacity dimension, and limit capacity. If A is such that $\underline{\dim}_B A = \overline{\dim}_B A$, the common value is denoted by $d := \dim_B A$, and we call it the box dimension of A . If, in addition to this, both $\mathcal{M}_*^d(A)$ and $\mathcal{M}^{*d}(A)$ are in $(0, \infty)$, we say that A is Minkowski nondegenerate. If, moreover, $\mathcal{M}_*^d(A) = \mathcal{M}^{*d}(A) =: \mathcal{M}^d(A) \in (0, \infty)$, then A is said to be Minkowski measurable.

Assume that A is such that $d := \dim_B A$ and $\mathcal{M}^d(A)$ exist. Then the value of $\mathcal{M}^d(A)^{-1}$ is called the lacunarity of A (B Mandelbrot, 1982). A bounded set $A \subset \mathbb{R}^N$ is said to be porous (A Denjoy, 1920) if there exist $\alpha > 0$ and $\delta > 0$ such that for every $x \in A$ and $r \in (0, \delta)$ there is $y \in \mathbb{R}^N$ such that the open ball $B_{\alpha r}(y)$ is contained in $B_r(x) \setminus A$. If A is porous then it is easy to see that $\underline{\dim}_B A < N$ (O Martio and M Vuorinen, 1987, A Salli, 1991).

We proceed with two examples. Let $A := C^{(a)}$, $a \in (0, 1/2)$, be the Cantor set obtained

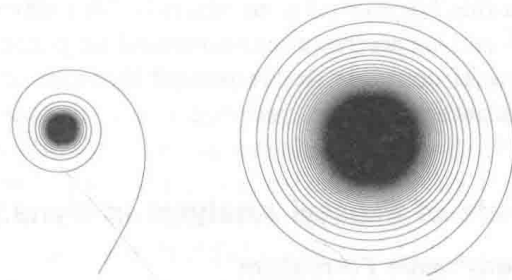


Figure 1 Spirals of equal box dimensions ($4/3$) and different lacunarities (0.43 and 0.05).

from $[0, 1]$ by consecutive deletion of 2^k middle open intervals of length $a^k(1 - 2a)$ in step $k \in \mathbb{N} \cup \{0\}$. Then $\dim_B A = (\log 2)/(\log(1/a))$ (G Bouligand, 1928), and A is nondegenerate, but not Minkowski measurable (Lapidus and Pomerance, 1993). For the spiral Γ of focus type defined by $r = m\varphi^{-\alpha}$ in polar coordinates, where $\alpha \in (0, 1)$ and $m > 0$ are fixed, $\varphi \geq \varphi_1 > 0$, we have $\dim_B \Gamma = 2/(1 + \alpha)$ (Y Dupain, M Mendés-France, C Tricot, 1983). It is Minkowski measurable (Žubrinčić and Županović, 2005), and the larger m , the smaller the lacunarity; see Figure 1.

Hausdorff Dimension

For a given subset A of \mathbb{R}^N (not necessarily bounded) and $s \geq 0$ we define $\mathcal{H}^s(A) := \lim_{\varepsilon \rightarrow 0} \inf \{\sum_{i=1}^{\infty} r_i^s \in [0, \infty]\}$, where the infimum is taken over all finite or countable coverings of A by open balls of radii $r_i \leq \varepsilon$. The value of $\mathcal{H}^s(A)$ is called s -dimensional Hausdorff outer measure of A . The Hausdorff dimension of A , sometimes called the Hausdorff–Besicovitch dimension, is defined by

$$\dim_H A := \inf\{s \geq 0 : \mathcal{H}^s(A) = 0\}$$

If A is bounded then $\dim_H A \leq \underline{\dim}_B A \leq \overline{\dim}_B A \leq N$.

We say that A is Hausdorff nondegenerate (or d -set) if $\mathcal{H}^d(A) \in (0, \infty)$ for some $d \geq 0$. Cantor sets share this property, and $\dim_H C^{(a)} = (\log 2)/(\log(1/a))$, where $a \in (0, 1/2)$ (Hausdorff, 1919).

Gauge Functions

The notions of Minkowski contents and Hausdorff measure can be generalized using gauge functions $h : [0, \varepsilon_0) \rightarrow \mathbb{R}$ that are assumed to be continuous, increasing, and $h(0) = 0$. For example,

$$\mathcal{M}^{*h}(A) := \overline{\lim}_{\varepsilon \rightarrow 0} \frac{|A_\varepsilon|}{\varepsilon^N} h(\varepsilon)$$

and similarly for $\mathcal{M}_*^h(A)$ (M Lapidus and C He, 1997), while for $\mathcal{H}^h(A)$ it suffices to change r_i^s with $h(r_i)$ in the above definition of the Hausdorff outer measure (Besicovitch, 1934). Gauge functions are used for sets that are Minkowski or Hausdorff

degenerate. The aim, if possible, is to find an explicit gauge function so that the corresponding generalized Minkowski contents or Hausdorff measure of A be nondegenerate.

Methods of Fractal Analysis in Dynamics

Thermodynamic Formalism

Thermodynamic formalism has been developed by Sinai (1972), Ruelle (1973), and Bowen (1975), using methods of statistical mechanics in order to study dynamics and to find dimensions of various fractal sets. We first describe a “dictionary” for explicit geometric constructions of Cantor-like sets. Let X_p be the set of all sequences $i = (i_1, i_2, \dots)$ of elements i_k from a given set of p symbols, say $\{1, 2, \dots, p\}$. We endow X_p with the metric $d(i, j) := \sum_k 2^{-k} |i_k - j_k|$ and introduce the one-sided shift operator (or left shift) $\sigma: X_p \rightarrow X_p$ defined by $(\sigma(i))_n = i_{n+1}$, that is, $\sigma(i_1, i_2, i_3, \dots) = (i_2, i_3, i_4, \dots)$. A set $Q \subseteq X_p$ is called the symbolic dynamics if it is compact and σ -invariant, that is, $\sigma(Q) \subseteq Q$. Hence, (Q, σ) is a symbolic dynamical system. Denote $i[n] := (i_1, \dots, i_n)$. Given a continuous function $\varphi: Q \rightarrow \mathbb{R}$, let us define the topological pressure of φ with respect to σ by

$$P(\varphi) := \lim_{n \rightarrow \infty} \frac{1}{n} \log \sum_{\{i[n]: i \in Q\}} E(i[n])$$

$$E(i[n]) := \exp \left(\sup_{\{j \in Q: j[n] = i[n]\}} \sum_{k=0}^{n-1} \varphi(\sigma^k(j)) \right)$$

The topological entropy of $\sigma|_Q$ is defined by $h(\sigma|_Q) := P(0)$, that is,

$$h(\sigma|_Q) = \lim_{n \rightarrow \infty} \frac{1}{n} \log \# \{i[n]: i \in Q\}$$

where $\#$ denotes the cardinal number of a set. The above function $\varphi_n := \sum_{k=0}^{n-1} \varphi \circ \sigma^k$ has the property $\varphi_{n+m} = \varphi_n + \varphi_m \circ \sigma^n$, and therefore we speak about additive thermodynamic formalism. Topological pressure was introduced by D Ruelle (1973) and extended by P Walters (1976). Bowen's equation (1979) has a very important role in the computation of the Hausdorff dimension of various sets. For the unknown $s \in \mathbb{R}$, and with a suitably chosen function φ , this equation reads

$$P(s\varphi) = 0$$

Geometric Constructions

A geometric construction (Q, Δ) in \mathbb{R}^m indexed by symbolic dynamics Q is a family Δ of compact sets

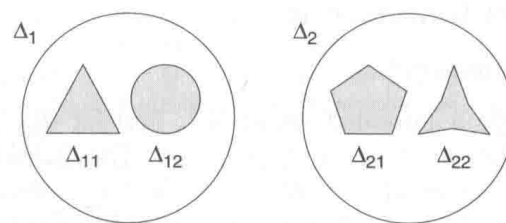


Figure 2 Cantor-like set.

$\Delta_{i[n]} \subset \mathbb{R}^m$, $i \in Q$, $n \in \mathbb{N}$, such that $\text{diam} \Delta_{i[n]} \rightarrow 0$ as $n \rightarrow \infty$, $\Delta_{i[n+1]} \subseteq \Delta_{i[n]}$, $\Delta_{i[n]} = \overline{\text{int} \Delta_{i[n]}}$ for every $i \in Q$ and all n , and $\text{int} \Delta_{i[n]} \cap \text{int} \Delta_{j[n]} = \emptyset$ whenever $i[n] \neq j[n]$ (Moran's open set condition). This family induces the Cantor-like set

$$F := \bigcap_{n=1}^{\infty} \left(\bigcup_{i \in Q} \Delta_{i[n]} \right)$$

(see Figure 2). The mapping $h: Q \rightarrow F$ defined by $h(i) := \bigcap_{n=1}^{\infty} \Delta_{i[n]}$ is called the coding map of F . The above geometric construction includes well-known iterated function systems of similarities as a special case. If $\lambda_1, \dots, \lambda_p$ are given numbers in $(0, 1)$, and $\Delta_{i[n]}$ are balls of radii $r_{i[n]} := \lambda_{i_1} \dots \lambda_{i_n}$, then $s := \dim_H F$ is the unique solution of Bowen's equation $P(s\varphi) = 0$, where φ is defined by $\varphi(i) := \log \lambda_{i_1}$ (Ya Pesin and H Weiss, 1996). In this case Bowen's equation is equivalent to Moran's equation (1946),

$$\sum_{k=1}^p \lambda_k^s = 1$$

This result has been generalized by L Barreira (1996) using the Carathéodory–Pesin construction (1988). Let us illustrate Barreira's theory of nonadditive thermodynamic formalism with a special case. Assume that (Q, Δ) is a geometric construction for which the sets $\Delta_{i[n]}$ are balls, and let there exist $\delta > 0$ such that $r_{i[n+1]} \geq \delta \cdot r_{i[n]}$ and $r_{i[n+m]} \leq r_{i[n]} r_{\sigma^n(i)[m]}$ for all $i \in Q$, $n, m \in \mathbb{N}$. Then $\dim_H F = \dim_B F = s$, where s is the unique real number such that

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log \sum_{\{i[n]: i \in Q\}} r_{i[n]}^s = 0 \quad [1]$$

This is a special case of Barreira's extension of Bowen's equation to nonadditive thermodynamic formalism. Moran's equation can be deduced from [1] by defining $r_{i[n]} := \lambda_{i_1} \dots \lambda_{i_n}$, where $i = (i_1, i_2, \dots)$, and $\lambda_1, \dots, \lambda_p \in (0, 1)$ are given numbers. Pesin and Weiss (1996) showed that Moran's open set condition can be weakened so that partial intersections of interiors of pairs of basic sets in the family Δ are allowed. Thermodynamic formalism has been used to study the Hausdorff dimension of Julia sets

(Ruelle, 1982), horseshoes (H McCluskey and A Manning, 1983), etc.

An important example of symbolic dynamics is the topological Markov chain X_A generated by a $p \times p$ matrix A with entries $a_{ij} \in \{0, 1\}$:

$$X_A := \{i = (i_1, i_2, \dots) \in X_p : a_{i_k i_{k+1}} = 1 \text{ for all } k \in \mathbb{N}\}$$

It is a compact, σ -invariant subset of X_p . The map $\sigma|_{X_A}$ is called the subshift of finite type (Bowen, 1975). A construction of Cantor-like set F using dynamics $Q = X_p$ is called a simple geometric construction, while a geometric construction is said to be a Markov geometric construction if $Q = X_A$. If F is obtained by a Markov geometric construction such that all $\Delta_{i[n]}$ are balls of radii $r_{i[n]} := \lambda_{i_1} \dots \lambda_{i_n}$, where $\lambda_{i_j} \in (0, 1)$, $i_j \in \{1, \dots, p\}$, then $\dim_B F = \dim_H F = s$, where s is the unique solution of equation $\rho(AM_s) = 1$. Here $M_s := \text{diag}(\lambda_1^s, \dots, \lambda_p^s)$ and $\rho(AM_s)$ is the spectral radius of the matrix AM_s . This and more general results have been obtained by Pesin and Weiss (1996).

Any Cantor-like set F obtained via iterated function system of similarities satisfying Moran's open set condition is Hausdorff nondegenerate (Moran, 1946). If F is of nonlattice type, that is, the set $\{\log \lambda_1, \dots, \log \lambda_p\}$ is not contained in $r \cdot \mathbb{Z}$ for any $r > 0$, then F is Minkowski measurable (D Gatzouras, 1999).

Hyperbolic Measures

Let X be a complete metric space and assume that $f: X \rightarrow X$ is continuous. Let μ be an f -invariant Borel probability measure on X (i.e., $\mu(f^{-1}(A)) = \mu(A)$ for measurable sets A) with a compact support. The Hausdorff dimension of μ , and the lower and upper box dimensions of μ (L-S Young, 1982) are defined by

$$\begin{aligned} \dim_H \mu &:= \inf\{\dim_H Z : Z \subseteq X, \mu(Z) = 1\} \\ \underline{\dim}_B \mu &:= \liminf_{\delta \rightarrow 0} \{\underline{\dim}_B Z : Z \subseteq X, \mu(Z) \geq 1 - \delta\} \\ \overline{\dim}_B \mu &:= \liminf_{\delta \rightarrow 0} \{\overline{\dim}_B Z : Z \subseteq X, \mu(Z) \geq 1 - \delta\} \end{aligned}$$

It is natural to introduce the lower and upper pointwise dimensions of μ at $x \in X$ by

$$\underline{d}_\mu(x) := \liminf_{r \rightarrow 0} \frac{\log \mu(B_r(x))}{\log r}$$

and similarly $\overline{d}_\mu(x)$. It has been shown by Young (1982) that if X has finite topological dimension and if μ is exact dimensional, that is, $\underline{d}_\mu(x) = \overline{d}_\mu(x) =: d$ for μ -a.e. $x \in X$, then

$$\dim_H \mu = \dim_B \mu = d$$

She also proved that hyperbolic measures (ergodic measures with nonzero Lyapunov exponents), invariant under a $C^{1+\alpha}$ -diffeomorphism, $\alpha > 0$, are exact dimensional. F Ledrappier (1986) derived exact dimensionality for hyperbolic Bowen–Ruelle–Sinai measures. This result was extended by Ya Pesin and Ch Yue (1996) to hyperbolic measures with semilocal product structure. J-P Eckmann and D Ruelle (1985) conjectured that the exact dimensionality holds for general hyperbolic measures, and this was proved by Barreira, Pesin, and Schmeling (1996). More precisely, if f is a $C^{1+\alpha}$ -diffeomorphism on a smooth Riemann manifold X without boundary, and if μ is f -invariant, compactly supported Borel probability measure, then its hyperbolicity implies that

$$\underline{d}_\mu(x) = \overline{d}_\mu(x) = d_\mu^s(x) + d_\mu^u(x)$$

for μ -a.e. $x \in X$, where $d_\mu^s(x)$ and $d_\mu^u(x)$ are stable and unstable pointwise dimensions of μ at x introduced by Ledrappier and Young (1985).

Multifractal Analysis of Functions and Measures

Invariant sets of many dynamical systems are not self-similar. Roughly speaking, the aim of multifractal analysis is to make a decomposition of the invariant set with respect to desired fractal properties and then to study a fractal dimension of each set of the decomposition. Some dynamical systems have invariant sets equal to graphs of Hölderian functions $f: \mathbb{R}^N \rightarrow \mathbb{R}$, so that wavelet methods can be used. One of the goals of multifractal analysis of functions is to study the spectrum of singularities of f defined by

$$d_f(\alpha) := \dim_H H_\alpha(f)$$

introduced by U Frisch and G Parisi (1985) in the context of fully developed turbulence. Here $H_\alpha(f)$ is the set of points at which the corresponding pointwise Hölder exponent of f is equal to $\alpha \geq 0$. If the function f is self-similar then $d_f(\alpha)$ is real analytic and strictly concave (first increasing and then decreasing) on an explicit interval $(\underline{a}, \overline{a})$ (S Jaffard, 1997). It is natural to consider the set $C_{\alpha, \beta}(f)$ of points x_0 called chirps of order (α, β) (Y Meyer 1996), at which f behaves roughly like $|x - x_0|^\alpha \sin(1/|x - x_0|^\beta)$, $\beta > 0$. The function $D_f(\alpha, \beta) := \dim_H C_{\alpha, \beta}(f)$ is called the chirp spectrum of f (S Jaffard 2000). Wavelet methods have found applications in the study of evolution equations and in modeling and detection of chirps in turbulent flows (S Jaffard, Y Meyer, RD Robert, 2001).

Basic ideas of multifractal analysis have been introduced by physicists T Halsey, MH Jensen,

LP Kadanoff, I Procaccia, and BI Shraiman (1988). In applications it often deals with an invariant ergodic probability measure associated with the dynamical system considered. Multifractal analysis of a Borel finite measure μ defined on \mathbb{R}^N consists in the study of the function

$$d_\mu(\alpha) := \dim_H K_\alpha(\mu), \quad \alpha \geq 0$$

called the spectrum of pointwise dimensions of μ . Here $K_\alpha(\mu)$ is the set of points where the pointwise dimension of μ is equal to α :

$$K_\alpha(\mu) := \{x \in \mathbb{R}^N : \underline{d}_\mu(x) = \bar{d}_\mu(x) = \alpha\}$$

It is also of interest to study the Hausdorff dimension of irregular set $K(\mu) := \{x \in \mathbb{R}^N : \underline{d}_\mu(x) < \bar{d}_\mu(x)\}$. These sets are pairwise disjoint and constitute a multifractal decomposition of \mathbb{R}^N , that is,

$$\mathbb{R}^N = K(\mu) \cup (\cup_{\alpha \in \mathbb{R}} K_\alpha(\mu))$$

The function $d_\mu(\alpha)$ provides an important information about the complexity of multifractal decomposition. In many situations, there is an open interval $(\underline{\alpha}, \bar{\alpha})$ on which the function $d_\mu(\alpha)$ is analytic and strictly concave (first increasing and then decreasing), and equal to the Legendre transform of an explicit convex function. We thus obtain an uncountable family of sets $K_\alpha(\mu)$ with positive Hausdorff dimension, which shows enormous complexity of the multifractal decomposition of \mathbb{R}^N . These and related questions have been studied by L Olsen (1995), K Falconer (1996), Pesin and Weiss (1996), Barreira and Schmeling (2000), and many other authors.

Local Lyapunov Dimension

Let Ω be an open set in \mathbb{R}^N and let $f: \Omega \rightarrow \mathbb{R}^N$ be a C^1 -map. To any fixed $x \in \Omega$ we assign N singular values $a_1 \geq a_2 \geq \dots \geq a_N \geq 0$ of f , defined as square roots of eigenvalues of the matrix $f'(x)^T \cdot f'(x)$, where $f'(x)$ is the Jacobian of f at x , and $f'(x)^T$ its transpose. The local Lyapunov dimension of f at x is defined by

$$\dim_L(f, x) := j + s$$

where j is the largest integer in $[0, N]$ such that $a_1 \cdot \dots \cdot a_j \geq 1$ (if there is no such j we let $j=0$), and $s \in [0, 1]$ is the unique solution of $a_1 \cdot \dots \cdot a_j a_{j+1}^s = 1$ (except for $j=N$, when we define $s=0$). This definition, due to BR Hunt (1996), is close to that of Kaplan and Yorke (1979). The Jacobian $f'(x)$ contracts k -dimensional volumes (that is, $a_1 \cdot \dots \cdot a_k < 1$) if and only if $\dim_L(f, x) < k$. In this case, we say that f is k -contracting at x . Furthermore, the function $x \mapsto \dim_L(f, x)$ is upper-semicontinuous, so that for

any compact subset A of Ω the Lyapunov dimension of f on A ,

$$\dim_L(f, A) := \max_{x \in A} \dim_L(f, x)$$

is well defined. Yu S Ilyashenko conjectured that if f locally contracts k -dimensional volumes then the upper box dimension of any compact invariant set is $< k$. Hunt (1996) proved that if A is a compact, strictly invariant set of f (i.e., $f(A) = A$) then

$$\overline{\dim}_B A \leq \dim_L(f, A) \quad [2]$$

This is an improvement of $\dim_H A \leq \dim_L(f, A)$ obtained by A Douady and J Oesterlé (1980), and independently by Ilyashenko (1982). MA Blinchevskaya and Yu S Ilyashenko (1999) proved that if A is any attractor of a smooth map in a Hilbert space that contracts k -dimensional volumes then $\overline{\dim}_B A \leq k$. See [3] below.

A continuous variant of this method is used in order to obtain estimates of fractal dimensions of global attractors of dynamical systems (X, S) on a Hilbert space X . Here $S(t), t \geq 0$, is a semigroup of continuous operators on X , that is, $S(t+s) = S(t)S(s)$ and $S(0) = I$. A set A in X is called a global attractor of dynamical system if it is compact, attracting (i.e., for any bounded set B and $\varepsilon > 0$ there exists t_0 such that for $t \geq t_0$ we have $S(t)B \subseteq A_\varepsilon$), and A is strictly invariant (i.e., $S(t)A = A$ for all $t \geq 0$).

Applications in Dynamics

Logistic Map

M Feigenbaum, a mathematical physicist, introduced and studied the dynamics of the logistic map $f_\lambda: [0, 1] \rightarrow [0, 1], f_\lambda(x) := \lambda x(1-x), \lambda \in (0, 4]$. Taking $\lambda = \lambda_\infty \approx 3.570$ the corresponding invariant set $A \subset [0, 1]$ (i.e., $S_1(A) \cup S_2(A) = A$, where S_i are two branches of f_λ^{-1}) has both Hausdorff and box dimensions equal to ≈ 0.538 (P Grassberger 1981, P Grassberger and I Procaccia, 1983). The set A has Cantor-like structure, but is not self-similar. Its multifractal properties have been studied by U Frisch, K Khanin, and T Matsumoto (2004).

Smale Horseshoe

In the early 1960s S Smale defined his famous horseshoe map and showed that it has a strange invariant set resulting in chaotic dynamics. The notion of strange attractor was introduced in 1971 by Ruelle and Takens in their study of turbulence. Let S be a square in the plane and let $f: \mathbb{R}^2 \rightarrow \mathbb{R}^2$ be a map transforming S as indicated in Figure 3, such that on both components of $S \cap f^{-1}(S)$ the map f is

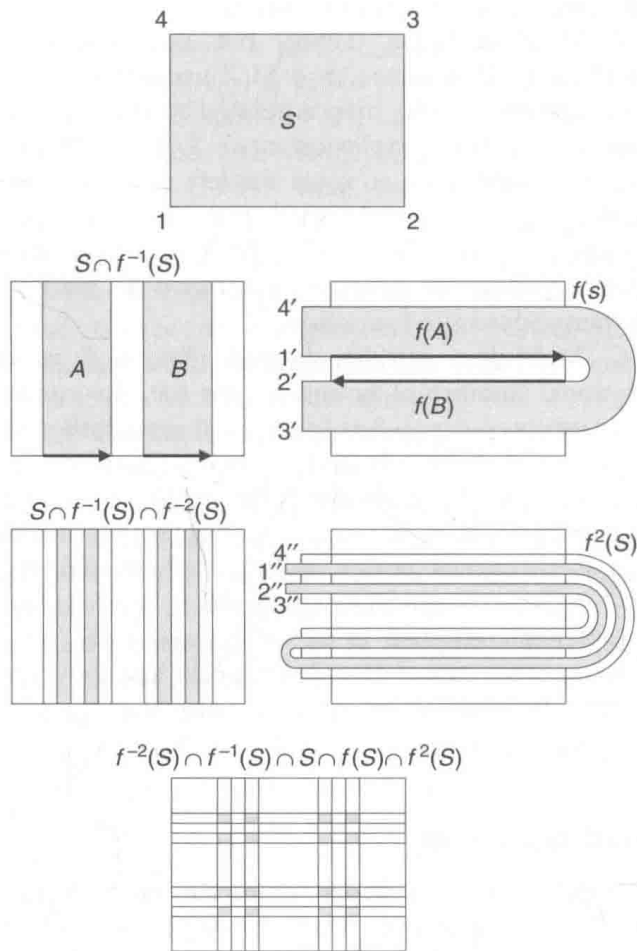


Figure 3 The Smale horseshoe.

affine and preserves both horizontal and vertical directions, and such that points 1, 2, 3, and 4 are mapped to $1', 2', 3',$ and $4'$. Iterating f we get backward invariant set $\Lambda_- := \bigcap_{i=0}^{\infty} f^{-i}(S)$, forward invariant set $\Lambda_+ := \bigcap_{i=0}^{\infty} f^i(S)$, and invariant set (horseshoe) $\Lambda_f := \Lambda_+ \cap \Lambda_-$. These sets have the Cantor set structure. More precisely, assuming that the contraction parameter of f in vertical direction is $a \in (0, 1/2)$, and the expansion parameter in horizontal direction is $b > 2$, then $\Lambda_+ = [0, 1] \times C^{(a)}$, where $C^{(a)}$ is the Cantor set, $\Lambda_- = C^{(1/b)} \times [0, 1]$, and $\Lambda_f = C^{(1/b)} \times C^{(a)}$, so that $\dim_B \Lambda_+ = \dim_H \Lambda_+ = 1 + (\log 2)/(\log(1/a))$ and

$$\dim_B \Lambda_f = \dim_H \Lambda_f = \frac{\log 2}{\log b} + \frac{\log 2}{\log(1/a)}$$

This is a special case of a general result about horseshoes in \mathbb{R}^2 (not necessarily affine), due to McCluskey and Manning (1983), stated in terms of the pressure function. Analogous result as above can be obtained for Smale solenoids. In \mathbb{R}^3 it is possible to construct affine horseshoes Λ_f such that $\dim_H \Lambda_f < \dim_B \Lambda_f$ (M Pollicott and H Weiss, 1994).

Smale discovered a connection between homoclinic orbits and the horseshoe map. It has been noticed that

fractal dimensions have important role in the study of homoclinic bifurcations of nonconservative dynamical systems. Since the 1970s the relationship between invariants of hyperbolic sets and the typical dynamics appearing in the unfolding of a homoclinic tangency by a parametrized family of surface diffeomorphisms has been studied by J Newhouse, J Palis, F Takens, J-C Yoccoz, C G Moreira and M Viana. The main result is that if the Hausdorff dimension of the hyperbolic set involved in the tangency is < 1 then the parameter set where the hyperbolicity prevails has full Lebesgue density. If the Hausdorff dimension is > 1 , then hyperbolicity is not prevalent. This result and its proof were inspired by previous work of J M Marstrand (1954) about arithmetic differences of Cantor sets on the real line. According to the result by Moreira, Palis, and Viana (2001) the paradigm “hyperbolicity prevails if and only if the Hausdorff dimension is < 1 ” extends to homoclinic bifurcations in any dimension.

Using methods of thermodynamic formalism McCluskey and Manning (1983) proved that if f is the above horseshoe map, then there exists a C^1 -neighborhood U of f such that the mapping $f \mapsto \dim_H \Lambda_f$ is continuous. Continuity of box and Hausdorff dimensions for horseshoes has been studied also by Takens, Palis, and Viana (1988).

Lorenz Attractor

EN Lorenz (1963), a meteorologist and student of G Birkhoff, showed by numerical experiments that for certain values of positive parameters σ, r, b , the quadratic system

$$\dot{x} = \sigma(y - x), \quad \dot{y} = rx - y - xz, \quad \dot{z} = xy - bz$$

has the global attractor A , for example, for $\sigma = 10$, $r = 28$, $b = 8/3$. In this case $\dim_B A \approx 2.06$, which is a numerical result (Grassberger and Procaccia, 1983). Using the analysis of local Lyapunov dimension along the flow in A , G A Leonov (2001) showed that if $\sigma + 1 \geq b \geq 2$ and $r\sigma^2(4 - b) + 2\sigma(b - 1) \times (2\sigma - 3b) > b(b - 1)^2$ then

$$\overline{\dim}_B A \leq 3 - \frac{2(\sigma + b + 1)}{\sigma + 1 + \sqrt{(\sigma - 1)^2 + 4r\sigma}}$$

Hénon Attractor

M Hénon (1976), a theoretical astronomer, discovered the map $f: \mathbb{R}^2 \rightarrow \mathbb{R}^2$, $f(x, y) := (a + by - x^2, x)$, capturing several essential properties of the Lorenz system. In the case of $a = 1.4$ and $b = 0.3$, Hunt (1996) derived from [2] that for any compact, strictly f -invariant set A in the trapping region $[-1.8, 1.8]^2$

there holds $\overline{\dim}_B A < 1.5$. Numerical experiments show that $\dim_B A \approx 1.28$ (Grassberger, 1983). Assuming $a > 0$, $b \in (0, 1)$, and $P_{\pm}(x_{\pm}, x_{\pm}) \in A$, where P_{\pm} are fixed points of f , Leonov (2001) obtained that

$$\overline{\dim}_B A \leq 1 + \frac{1}{1 - \ln b / \ln(\sqrt{x_-^2 + b} - x_-)}$$

Here

$$x_{\pm} := \frac{1}{2} \left[b - 1 \pm \sqrt{(b - 1)^2 + 4a} \right]$$

The proof is based on the study of local Lyapunov dimension of f and its iterates on A .

Embedology

The physical relevance of box dimensions in the study of attractors is related to the problem of finding the smallest possible dimension n sufficient to “embed” an attractor into \mathbb{R}^n . If $A \subset \mathbb{R}^k$ is a compact set and if $n > 2\overline{\dim}_B A$, then almost every map from \mathbb{R}^k into \mathbb{R}^n , in the sense of prevalence, is one-to-one on A and, moreover, it is an embedding on smooth manifolds contained in A (T Sauer, J A Yorke, and M Casdagli, 1991). If A is a strange attractor then the same is true for almost every delay-coordinate map from \mathbb{R}^k to \mathbb{R}^n . This improves an earlier result by H Whitney (1936) and F Takens (Takens’ embedology, 1981). The above notion of prevalence means the following: a property holds almost everywhere in the sense of prevalence if it holds on a subset S of the space $V := C^1(\mathbb{R}^k, \mathbb{R}^n)$ for which there exists a finite-dimensional subspace $E \subset V$ (probe space) such that for each $v \in V$ we have that $v + e \in S$ for Lebesgue a.e. $e \in E$.

Julia and Mandelbrot Sets

M Shishikura (1998) proved that the boundary of the Mandelbrot set M generated by $f_c(z) := z^2 + c$ has the Hausdorff dimension equal to 2, thus answering positively to the conjecture by B Mandelbrot, J Milnor, and other mathematicians. Also for Julia sets there holds $\dim_H J(f_c) = 2$ for generic c in M (i.e., on the set of second Baire category). The proof is based on the study of the bifurcation of parabolic periodic points. Also, each baby Mandelbrot set sitting inside of M has the boundary of Hausdorff dimension 2 (L Tan, 1998). Shishikura’s results hold for more general functions $f(z) := z^d + c$, where $d \geq 2$.

For Julia sets $J(f_c)$ generated by $f_c(z) := z^2 + c$ there holds $d(c) := \dim_H J(f_c) = 1 + |c|^2 / (4 \log 2) + o(|c|^2)$ for $c \rightarrow 0$. This and more general results have been obtained by Ruelle (1982). He also proved that the function $d(c)$ when restricted to the interval $[0, \infty)$ is real analytic in $[0, 1/4) \cup (1/4, \infty)$.

Furthermore, it is left continuous at $1/4$ (O Bodart and M Zinsmeister, 1996), but not continuous (A Douady, P Sentenac, and M Zinsmeister, 1997). Discontinuity of this map is related to the phenomenon of parabolic implosion at $c = 1/4$. The derivative $d'(c)$ tends to $+\infty$ from the left at $c = 1/4$ like $(1/4 - c)^{d(1/4)-3/2}$ (G Havard and M Zinsmeister, 2000). Here $d(1/4) \approx 1.07$, which is a numerical result. Analysis of dimensions is based on methods of thermodynamic formalism.

C McMullen (1998) showed that if θ is an irrational number of bounded type (i.e., its continued fractional expansion $[a_1, a_2, \dots]$ is such that the sequence (a_i) is bounded from above) and $f(z) := z^2 + e^{2\pi\theta i} z$, then the Julia set $J(f)$ is porous. In particular, $\overline{\dim}_B J(f) < 2$. Y C Yin (2000) showed that if all critical points in $J(f)$ of a rational map $f: \mathbb{C} \rightarrow \mathbb{C}$ are nonrecurrent (a point is nonrecurrent if it is not contained in its ω -limit set) then $J(f)$ is porous, hence $\overline{\dim}_B J(f) < 2$. Urbański and Przytycki (2001) described more general rational maps such that $\overline{\dim}_B J(f) < 2$.

Spiral Trajectories

A standard planar model where the Hopf–Takens bifurcation occurs is $\dot{r} = r(r^{2l} + \sum_{i=0}^{l-1} a_i r^{2i})$, $\dot{\phi} = 1$, where $l \in \mathbb{N}$. If Γ is a spiral tending to the limit cycle $r = a$ of multiplicity m (i.e., $r = a$ is a zero of order m of the right-hand side of the first equation in the system) then $\dim_B \Gamma = 2 - 1/m$. Furthermore, for $m > 1$ the spiral is Minkowski measurable (Žubrinčić and Županović, 2005). For $m = 1$ the spiral is Minkowski nondegenerate with respect to the gauge function $h(\varepsilon) := \varepsilon(\log(1/\varepsilon))^{-1}$.

Infinite-Dimensional Dynamical Systems

In many situations the dynamics of the global attractor A of the flow corresponding to an autonomous Navier–Stokes system is finite-dimensional (Ladyzhenskaya, 1972). This means that there exists a positive integer N such that any trajectory in A is completely determined by its orthogonal projection onto an N -dimensional subspace of a Hilbert space X . The aim is to find estimates of box and Hausdorff dimensions of the global attractor, in order to understand some of the basic and challenging problems of turbulence theory. If A is a subset of a Hilbert space X , its Hausdorff dimension is defined analogously as for $A \subset \mathbb{R}^N$. The definition of the upper box dimension can be extended from $A \subset \mathbb{R}^N$ to

$$\overline{\dim}_B A := \lim_{\varepsilon \rightarrow 0} \frac{\log m(A, \varepsilon)}{\log(1/\varepsilon)} \quad [3]$$

where $m(A, \varepsilon)$ is the minimal number of balls sufficient to cover a given compact set $A \subset X$. The value of $\log m(A, \varepsilon)$ is called ε -entropy of A .

Foias and Temam (1979), Ladyzhenskaya (1982), A V Babin and MI Vishik (1982), Ruelle (1983), and E Lieb (1984) were among the first who obtained explicit upper bounds of Hausdorff and box dimensions of attractors of infinite-dimensional systems. For global attractors A associated with some classes of two-dimensional Navier–Stokes equations with nonhomogeneous boundary conditions it can be shown that $\overline{\dim}_B A \leq c_1 G + c_2 Re^{3/2}$, where G is the Grashof number, Re is the Reynolds number, and c_i are positive constants (RM Brown, PA Perry, and Z Shen, 2000). VV Chepyzhov and AA Ilyin (2004) obtained that $\overline{\dim}_B A \leq (1/\sqrt{2\pi})(\lambda_1|\Omega|)^{1/2}G$ for equations with homogeneous boundary conditions, where $\Omega \subset \mathbb{R}^2$ is a bounded domain, and λ_1 is the first eigenvalue of $-\Delta$. In the case of periodic boundary conditions Constantin, Foias, and Temam (1988) proved that $\overline{\dim}_B A \leq c_1 G^{2/3}(1 + \log G)^{1/3}$, while for a special class of external forces there holds $\dim_H A \geq c_2 G^{2/3}$ (VX Liu, 1993). Let us mention an open problem by VI Arnol'd: is it true that the Hausdorff dimension of any attracting set of the Navier–Stokes equation on two-dimensional torus is growing with the Reynolds number?

In their study of partial regularity of solutions of three-dimensional Navier–Stokes equations, L Caffarelli, R Kohn, and L Nirenberg (1982) proved that the one-dimensional Hausdorff measure in space and time (defined by parabolic cylinders) of the singular set of any “suitable” weak solution is equal to zero. A weak solution is said to be singular at a point (x_0, t_0) if it is essentially unbounded in any of its neighborhoods. Dimensions of attractors of many other classes of partial differential equations (PDEs) have been studied, like for reaction–diffusion systems, wave equations with dissipation, complex Ginzburg–Landau equations, etc. Related questions for non-autonomous PDEs have been considered by VV Chepyzhov and MI Vishik since 1992.

Probability

Important examples of trajectories appearing in physics are provided by Brownian motions. Brownian motions ω in \mathbb{R}^N , $N \geq 2$, have paths $\omega([0, 1])$ of Hausdorff dimension 2 with probability 1, and they are almost surely Hausdorff degenerate, since $\mathcal{H}^2(\omega([0, 1])) = 0$ for a.e. ω (SJ Taylor, 1953). Defining gauge functions $b(\varepsilon) := \varepsilon^2 \log(1/\varepsilon) \times \log \log \log(1/\varepsilon)$ when $N = 2$, and $b(\varepsilon) := \varepsilon^2 \log(1/\varepsilon)$

when $N \geq 3$, there holds $\mathcal{H}^b(\omega([0, 1])) \in (0, \infty)$ for a.e. ω (D Ray, 1963, SJ Taylor, 1964). If $N = 1$ then a.e. ω has the box and Hausdorff dimensions of the graph of $\omega|_{[0, 1]}$ equal to $3/2$ (Taylor, 1953), and for the gauge function $b(\varepsilon) := \varepsilon^{3/2} \log \log(1/\varepsilon)$ the corresponding generalized Hausdorff measure is nondegenerate. In the case of $N \geq 2$ we have the uniform dimension doubling property (R Kaufman, 1969). This means that for a.e. Brownian motion ω there holds $\dim_H \omega(A) = 2 \dim_H A$ for all subsets $A \subset [0, \infty)$. There are also results concerning almost sure Hausdorff dimension of double, triple, and multiple points of a Brownian motion and of more general Lévy stable processes.

Fractal dimensions also appear in the study of stochastic differential equations, like

$$dx_t = X_0(x_t) dt + \sum_{k=1}^d X_k(x_t) d\theta_k(t), \quad x_0 = x \in \mathbb{R}^N$$

The stochastic flow $(x_t)_{t \geq 0}$ in \mathbb{R}^N is driven by a Brownian motion $(\theta(t))_{t \geq 0}$ in \mathbb{R}^d . Let us assume that $X_k, k = 0, \dots, d$, are C^∞ -smooth T -periodic divergence-free vector fields on \mathbb{R}^N . Then for almost every realization of the Brownian motion $(\theta(t))_{t \geq 0}$, the set of initial points x generating the flow $(x_t)_{t \geq 0}$ with linear escape to infinity (i.e., $\lim_{t \rightarrow \infty} (|x_t|/t) > 0$) is dense and of full Hausdorff dimension N (D Dolgopyat, V Kaloshin, and L Koralov, 2002).

Other Directions

There are many other fractal dimensions important for dynamics, like the Rényi spectrum for dimensions, correlation dimension, information dimension, Hentschel–Procaccia spectrum for dimensions, packing dimension, and effective fractal dimension. Relations between dimension, entropy, Lyapunov exponents, Gibbs measures, and multifractal rigidity have been investigated by Pesin, Weiss, Barreira, Schmeling, etc. Fractal dimensions are used to study dynamics appearing in Kleinian groups (D Sullivan, CJ Bishop, PW Jones, C McMullen, BO Stratmann, etc.), quasiconformal mappings and quasiconformal groups (FW Gehring, J Väisälä, K Astala, CJ Bishop, P Tukia, JW Anderson, P Bonfert-Taylor, EC Taylor, etc.), graph directed Markov systems (RD Mauldin, M Urbański, etc.), random walks on fractal graphs (J Kigami, A Telcs, etc.), billiards (H Masur, Y Cheung, P Bálint, S Tabachnikov, N Chernov, D Szász, IP Tóth, etc.), quantum dynamics (J-M Barbaroux, J-M Combes, H Schulz-Baldes, I Guarneri, etc.), quantum gravity (M Aizenman, A Aharony, ME Cates, TA Witten, GF Lawler, B Duplantier, etc.), harmonic analysis (RS Strichartz, ZM Balogh, JT Tyson, etc.),

number theory (L Barreira, M Pollicott, H Weiss, B Stratmann, B Saussol, etc.), Markov processes (R M Blumenthal, R Getoor, S J Taylor, S Jaffard, C Tricot, Y Peres, Y Xiao, etc.), and theoretical computer science (B Ya Ryabko, L Staiger, J H Lutz, E Mayordomo, etc.), and so on.

See also: Bifurcations of Periodic Orbits; Chaos and Attractors; Dissipative Dynamical Systems of Infinite Dimension; Dynamical Systems in Mathematical Physics: An Illustration from Water Waves; Ergodic Theory; Generic Properties of Dynamical Systems; Holomorphic Dynamics; Homoclinic Phenomena; Hyperbolic Dynamical Systems; Image Processing: Mathematics; Lyapunov Exponents and Strange Attractors; Partial Differential Equations: Some Examples; Polygonal Billiards; Quantum Ergodicity and Mixing of Eigenfunctions; Stochastic Differential Equations; Synchronization of Chaos; Universality and Renormalization; Wavelets: Applications; Wavelets: Mathematical Theory.

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Fractional Quantum Hall Effect

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Introduction

Interacting particles sometimes collectively behave in ways that take us by complete surprise. In a superfluid ^4He atoms flow without viscosity, and in a superconductor electrons flow without resistance. Such behaviors announce emergent structures and principles which have often found applications in other areas. This article concerns the surprising collective effects that occur when electrons are confined in two dimensions and subjected to a strong transverse magnetic field. At low temperatures, the Hall resistance (defined

below) exhibits plateaus on which it is precisely quantized at

$$R_H = \frac{h}{fe^2} \quad [1]$$

where h and e are fundamental constants and f is a plateau-specific rational fraction. This phenomenon is known as the “fractional quantum Hall effect” (FQHE), or, after its discoverers, the “Tsui–Stormer–Gossard” (TSG) effect. The underlying state provides a new paradigm for collective behavior in nature, and is understood in terms of a new class of quasiparticles known as “composite fermions,” which are topological bound states of electrons and quantized vortices. This article will outline the basics of the experimental phenomenology and our theoretical understanding of this effect.

The Hall Effect

The Ohm's law, $I = V/R$, tells us that the current through a resistor is proportional to the applied voltage. The local form of the law is

$$\mathbf{J} = \sigma \mathbf{E} \quad [2]$$

where σ is the conductivity, and $\mathbf{J} = q\rho\mathbf{v}$ is the current density for particles of charge q and density ρ moving with a velocity \mathbf{v} .

In 1879, E H Hall discovered that in the presence of a crossed electric and magnetic fields (\mathbf{E} and \mathbf{B}), the current flows in a direction "perpendicular" to the plane containing the two fields. Alternatively, the passage of current induces a voltage perpendicular to the direction of the current flow. This is known as the Hall effect (see Figure 1). The phenomenon has a classical origin. A consequence of the Lorentz force law of electrodynamics,

$$\mathbf{F} = q\left(\mathbf{E} + \frac{1}{c}\mathbf{v} \times \mathbf{B}\right) \quad [3]$$

which gives the force on a particle of charge q moving with a velocity \mathbf{v} , is that for crossed electric and magnetic fields the particle drifts in the direction $\mathbf{E} \times \mathbf{B}$ with a velocity $\mathbf{v} = c\mathbf{E}/B$. The current density is therefore given by $\mathbf{J} = q\rho\mathbf{v}$, where ρ is the (three-dimensional) density of particles. That produces the Hall resistivity

$$\rho_H = \frac{E_y}{J_x} = \frac{B}{\rho qc} \quad [4]$$

The von Klitzing Effect

Molecular beam epitaxy allows controllable layer by layer growth in which one type of semiconductor, say GaAs, can be grown on top of another, say $\text{Al}_x\text{Ga}_{1-x}\text{As}$, to produce an atomically sharp interface. By appropriately doping such structures, electrons can

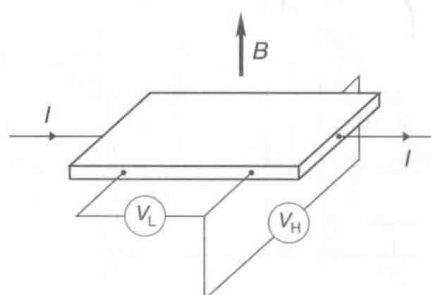


Figure 1 Schematics of magnetotransport measurement. I , V_L , and V_H are the current, longitudinal voltage, and the Hall voltage, respectively. The longitudinal and Hall resistances are defined as $R_L \equiv V_L/I$ and $R_H \equiv V_H/I$.

be captured at the interface, thus producing a two-dimensional electron system (2DES). We note that these are three-dimensional electrons confined to move in two dimensions. The interaction has the standard Coulomb form $V(r) = e^2/\epsilon r$, where ϵ is the dielectric constant of the host material. (In a hypothetical world which has only two space dimensions, the interaction would be logarithmic.)

The "integral quantum Hall effect" (IQHE) or the "von Klitzing effect" was discovered unexpectedly by von Klitzing and collaborators in 1980, in their study of Hall effect in a 2DES. In two dimensions, one defines the Hall resistance as

$$R_H = \frac{V_H}{I} \quad [5]$$

which, from classical electrodynamics, is expected to be proportional to the magnetic field B . That is indeed the case at small magnetic fields. At sufficiently high B , however, quantum mechanical effects appear in a dramatic manner. The essential observations are as follows.

1. When plotted as a function of the magnetic field B , the Hall resistance exhibits numerous plateaus. On any given plateau, R_H is precisely quantized with values given by

$$R_H = \frac{h}{ne^2} \quad [6]$$

where n is an integer (hence the name "integral quantum Hall effect"). The plateau occurs in the vicinity of $\nu \equiv Be/\rho hc = n$, where ν is the "filling factor" (defined below).

2. In the plateau region, the longitudinal resistance exhibits an Arrhenius behavior:

$$R_L \sim \exp\left(-\frac{\Delta}{2k_B T}\right) \quad [7]$$

This gives a filling-factor dependent energy scale Δ , which indicates the presence of a gap in the excitation spectrum. R_L vanishes in the limit $T \rightarrow 0$.

The absolute accuracy of the quantization has been established to a few parts in 10^8 for 1σ uncertainty, and the relative accuracy to a few parts in 10^{10} . There is presently no known "intrinsic" correction to the quantization. Perhaps, the most remarkable aspect of the effect is its universality. It is independent of the sample type, geometry, various material parameters (the band mass of the electron or the dielectric constant of the semiconductor), and disorder. The combination h/e^2 also occurs in the definition of the fine

structure constant $\alpha = e^2/\hbar c$, the value of which is approximately $1/137$. The Hall effect measurements in dirty, solid state systems thus provide one of the most accurate values for α . Finally, the lack of resistance at $T=0$ is to be contrasted with ordinary metals, for which the resistance at $T \rightarrow 0$, called the residual resistance, is finite and proportional to disorder.

The TSG Effect

The next revolution occurred in 1982 with the discovery of the TSG effect, that is, plateaus on which the Hall resistance is quantized at values given by eqn [1] (see Figure 2). The observation of the $R_H = h/fe^2$ plateau is often referred to as the observation of the fraction f . Improvement of experimental conditions has led to the observation of a large number of fractions over the years, revealing the richness of the TSG effect. At the time of the writing of this article, the number of observed fractions is more than 50 if one counts only fractions below unity. As in the von Klitzing effect, the longitudinal resistance exhibits an Arrhenius behavior, vanishing in the limit $T \rightarrow 0$.

Landau Levels

The Hamiltonian for a nonrelativistic electron moving in two space dimensions in a perpendicular magnetic field is given by

$$H = \frac{1}{2m_b} \left(\mathbf{p} + \frac{e\mathbf{A}}{c} \right)^2 \quad [8]$$

Here, m_b is the electron's band mass and $-e$ its charge. For a uniform magnetic field, the vector potential \mathbf{A} satisfies

$$\nabla \times \mathbf{A} = B\hat{z} \quad [9]$$

Because \mathbf{A} is a linear function of the spatial coordinates, it follows that H is a generalized two-dimensional harmonic oscillator Hamiltonian which is quadratic in both the spatial coordinates and in the canonical momentum $\mathbf{p} = -i\hbar\nabla$, and therefore can be diagonalized exactly.

A convenient gauge choice is the symmetric gauge:

$$\mathbf{A} = \frac{\mathbf{B} \times \mathbf{r}}{2} = \frac{B}{2}(-y, x, 0) \quad [10]$$

With the magnetic length $\ell = \sqrt{\hbar c/eB}$ and the cyclotron energy $\hbar\omega_c = \hbar eB/m_b c$ chosen as the

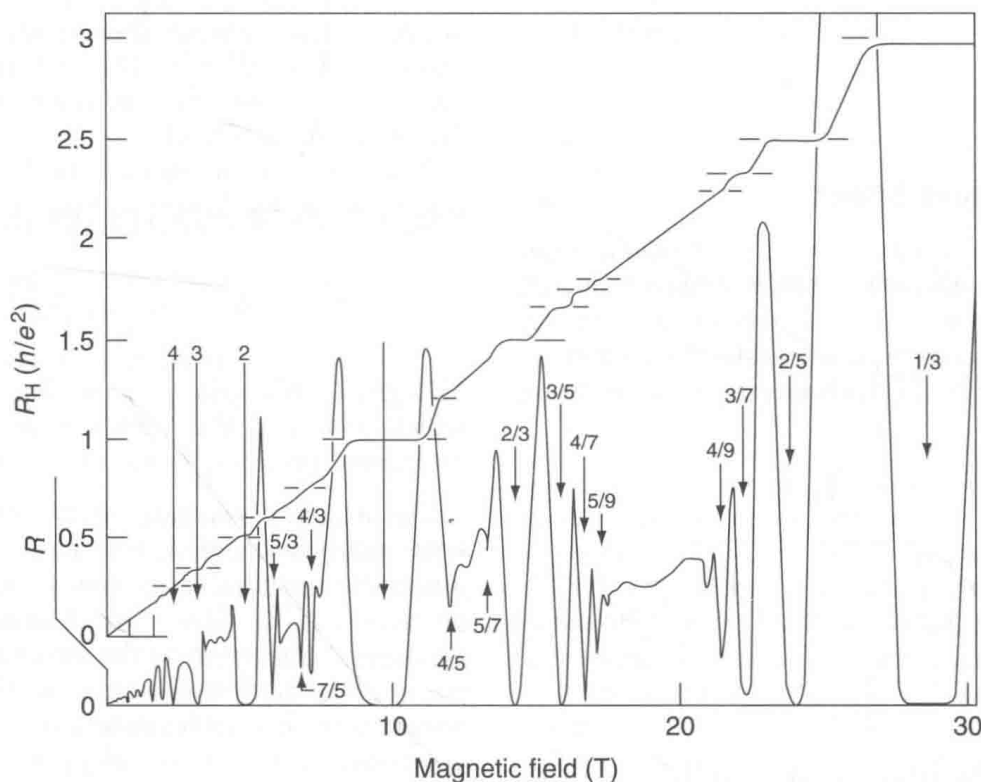


Figure 2 The TSG effect. The Hall resistance (R_H) exhibits many precisely quantized plateaus, concurrent with minima in the longitudinal resistance (R). Reproduced with permission from *Perspectives in Quantum Hall Effects*; HL Stormer and DC Tsui; SD Sarma and A Pinczuk (eds.); Copyright © 1997, Wiley. Reprinted with permission of John Wiley & Sons, Inc.

units for length and energy, the Hamiltonian can be expressed as

$$H = \frac{1}{2} \left[\left(-i \frac{\partial}{\partial x} - \frac{y}{2} \right)^2 + \left(-i \frac{\partial}{\partial y} + \frac{x}{2} \right)^2 \right] \quad [11]$$

Choosing as independent variables

$$z \equiv x - iy, \quad \bar{z} \equiv x + iy \quad [12]$$

we get

$$H = \frac{1}{2} \left(-4 \frac{\partial^2}{\partial z \partial \bar{z}} + \frac{1}{4} z \bar{z} - z \frac{\partial}{\partial z} + \bar{z} \frac{\partial}{\partial \bar{z}} \right) \quad [13]$$

Now define the following sets of ladder operators:

$$b = \frac{1}{\sqrt{2}} \left(\frac{\bar{z}}{2} + 2 \frac{\partial}{\partial z} \right) \quad [14]$$

$$b^\dagger = \frac{1}{\sqrt{2}} \left(\frac{z}{2} - 2 \frac{\partial}{\partial \bar{z}} \right) \quad [15]$$

$$a^\dagger = \frac{1}{\sqrt{2}} \left(\frac{\bar{z}}{2} - 2 \frac{\partial}{\partial z} \right) \quad [16]$$

$$a = \frac{1}{\sqrt{2}} \left(\frac{z}{2} + 2 \frac{\partial}{\partial \bar{z}} \right) \quad [17]$$

which have the property that

$$[a, a^\dagger] = 1, \quad [b, b^\dagger] = 1 \quad [18]$$

and all the other commutators are zero. In terms of these operators, the Hamiltonian can be written as

$$H = a^\dagger a + \frac{1}{2} \quad [19]$$

The eigenvalue of $a^\dagger a$ is an integer, n , called the Landau level (LL) index. The z -component of the canonical angular momentum operator, the only relevant component for the two-dimensional problem, is defined as

$$L_z = -i \frac{\partial}{\partial \theta} = \bar{z} \frac{\partial}{\partial \bar{z}} - z \frac{\partial}{\partial z} = a^\dagger a - b^\dagger b \quad [20]$$

Exploiting the property $[H, L_z] = 0$, the eigenfunctions will be chosen to diagonalize H and L_z simultaneously. The eigenvalue of L_z will be denoted by $-m$. The analogy to the Harmonic oscillator problem immediately gives the solution

$$H|m, n\rangle = E_n|m, n\rangle \quad [21]$$

where

$$E_n = \left(n + \frac{1}{2} \right) \quad [22]$$

and

$$|m, n\rangle = \frac{(b^\dagger)^{m+n} (a^\dagger)^n}{\sqrt{(m+n)!} \sqrt{n!}} |0, 0\rangle \quad [23]$$

where $m = -n, -n+1, \dots$. The single-particle orbital at the bottom of the two ladders defined by the two sets of raising and lowering operators is

$$\langle r|0, 0\rangle \equiv \eta_{0,0}(r) = \frac{1}{\sqrt{2\pi}} e^{-z\bar{z}/4} \quad [24]$$

which satisfies

$$a|0, 0\rangle = b|0, 0\rangle = 0 \quad [25]$$

The single-particle states are particularly simple in the lowest Landau level ($n=0$):

$$\eta_{0,m}(r) = \langle r|0, m\rangle = \frac{z^m e^{-z\bar{z}/4\ell^2}}{\sqrt{2\pi\ell^2 2^m m!}} \quad [26]$$

Aside from the ubiquitous Gaussian factor, a general state in the lowest Landau level is given by a polynomial of z ; it does not involve any \bar{z} . In other words, apart from the Gaussian factor, the lowest Landau level wave functions are analytic functions of z .

Landau Level Degeneracy

The state $\eta_{0,m}(r)$ is peaked strongly at $r = \sqrt{2m}\ell$. Neglecting order-1 effects, there are m states in the lowest Landau level in a disk of radius $r = \sqrt{2m}\ell$, giving a degeneracy of $(2\pi\ell^2)^{-1}$ per unit area per Landau level. (The same degeneracy is obtained for higher Landau levels as well.) It is equal to B/ϕ_0 , where $\phi_0 = hc/e$ is called the flux quantum, that is, there is one state per flux quantum in each Landau level.

Filling Factor

The number of filled Landau levels, called the filling factor, is given by

$$\nu = \rho 2\pi\ell^2 = \frac{\rho\phi_0}{B} \quad [27]$$

The Origin of Plateaus

The von Klitzing effect can be explained in terms of a model which neglects the interactions between electrons. It occurs because the ground state at an integral filling is unique and nondegenerate, separated from excitations by a gap. Laughlin (1981) showed that the disorder-induced Anderson localization also plays a crucial role in the establishment of the Hall plateaus. To see this, imagine changing the filling away from an integer by adding some

electrons or holes. In a perfect system, the additional particles would also be free to carry current, but in the actual, disordered sample, they are immobilized by impurities (which create localized states in the energy gap), and do not contribute to transport. The transport properties therefore remain unaffected as the filling factor is varied slightly away from an integer, and the system continues to behave as though it had filled shells.

The Lowest Landau Level Problem

The TSG effect arises due to interelectron interaction. We wish to obtain solutions for the Schrödinger equation

$$H\Psi = E\Psi \quad [28]$$

at an arbitrary filling ν , where

$$H = \sum_j \frac{1}{2m_b} \left[\frac{\hbar}{i} \nabla_j + \frac{e}{c} \mathbf{A}(\mathbf{r}_j) \right]^2 + \frac{e^2}{\epsilon} \sum_{j < k} \frac{1}{|\mathbf{r}_j - \mathbf{r}_k|} \quad [29]$$

The first term on the right-hand side is the kinetic energy in the presence of a constant external magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$, and the second term is the Coulomb interaction energy. (The Zeeman energy is not included explicitly because we consider, for now, magnetic fields that are sufficiently high that only fully spin-polarized states are relevant.) It is convenient to consider the limit $(e^2/\epsilon\ell)/(\hbar\omega_c) \rightarrow 0$, when the Coulomb interaction is so weak that it is not able to cause Landau level mixing, so electrons can be taken to be within the lowest Landau level. The kinetic energy then is an irrelevant constant which can be thrown away, and the Hamiltonian reduces to

$$H = \mathcal{P}_{\text{LLL}} \frac{e^2}{\epsilon} \sum_{j < k} \frac{1}{|\mathbf{r}_j - \mathbf{r}_k|} \mathcal{P}_{\text{LLL}} \quad [30]$$

“which must be solved with the lowest LL restriction,” as explicitly indicated by the lowest LL projection operator \mathcal{P}_{LLL} . The problem is thus mathematically well defined, but requires degenerate perturbation theory in an enormously large Hilbert space, with $\binom{N/\nu}{N}$ many particle basis vectors. The usual perturbative techniques are not useful due to the absence of a small parameter in the problem; $e^2/\epsilon\ell$ merely sets the energy scale in the lowest Landau level.

Composite-Fermion Theory

Inspired by the qualitative similarity between the integral and the fractional Hall effects, the composite-

fermion (CF) theory (Jain 1989) postulates that the eigenfunctions of interacting electrons at filling factor ν , Ψ_ν , are related to the (known) eigenfunctions of *non*interacting electrons at filling factor ν^* , Φ_{ν^*} , according to

$$\Psi_\nu = \mathcal{P}_{\text{LLL}} \Phi_{\nu^*} \prod_{j < k} (z_j - z_k)^{2p} \quad [31]$$

where \mathcal{P}_{LLL} denotes projection of the wave function on its right into the lowest Landau level. The filling factors are related by

$$\nu = \frac{\nu^*}{2p\nu^* + 1} \quad [32]$$

which can be seen as follows: the largest power of z_1 in Φ_{ν^*} (neglecting order-one corrections) is N/ν^* , as follows from the definition of the filling factor. The largest power of z_1 on the right-hand side is therefore $pN(N-1) + N/\nu^*$. This is the number of flux quanta penetrating the “sample.” Dividing it by N and taking the limit $N \rightarrow \infty$ gives the inverse of the filling factor ν^{-1} . These wave functions are now known to capture the correct nonperturbative physics of the TSG effect (see below), and also to provide extremely accurate representations for the actual correlated ground states and their excitations. They recover Laughlin’s 1983 wave function for the ground state at $\nu = 1/(2p+1)$, while clarifying that it is a part of a much bigger conceptual structure.

Physical Interpretation

The crucial property of the wave function in eqn [31] is that the complex Jastrow factor $\prod_{j < k} (z_j - z_k)^{2p}$ binds $2p$ vortices on each electron. More precisely, each electron sees $2p$ vortices on every other electron, in that a complete loop of an electron around any other electron produces a phase of $2\pi \times 2p$. The bound state is interpreted as a particle, called the “composite fermion.” Because the vortex is a topological object, so is the composite fermion. The vorticity $2p$ is quantized to be an even integer, as required by the single-valuedness and antisymmetry requirements of quantum mechanics, which will be seen to lie at the root of the exact quantization of the Hall resistance.

When composite fermions move about, they experience, in addition to the Aharonov–Bohm (AB) phase, also the Berry phases coming from vortices on other composite fermions. Imagine taking a composite fermion in a closed loop enclosing an area A . The phase associated with that loop is given by

$$\Phi^* = -2\pi \frac{BA}{\phi_0} + 2\pi 2p N_{\text{enc}} \quad [33]$$

where N_{enc} is the number of composite fermions inside the loop. The first term is the familiar AB phase due to a charge going around in a loop. The second is the Berry phase due to $2p$ vortices going around N_{enc} particles, with each particle producing a phase of 2π . Replacing N_{enc} by its average value ρA shows that, on average, Φ^* is equal to the AB phase from an “effective” magnetic field

$$B^* = B - 2p\rho\phi_0 \quad [34]$$

The composite fermions thus experience an effective magnetic field B^* which is much smaller than the external, applied field B . That lies at the heart of the phenomenology of this lowest Landau level liquid. One treats composite fermions as noninteracting in the simplest approximation. They form their own Landau-like levels in B^* . Their filling factor is defined as $\nu^* = \rho\phi_0/B^*$, with which eqn [34] becomes equivalent to eqn [32]. The effective field B^* can be antiparallel to B , in which case $\nu^* = \rho\phi_0/B^*$ is formally negative. For negative values of ν^* , Φ_{ν^*} in eqn [31] is defined as $\Phi_{-|\nu^*|} = [\Phi_{|\nu^*|}]^*$, because complex conjugation is equivalent to switching the direction of the magnetic field.

Fermion Chern–Simons Theory

Lopez and Fradkin (1991) developed a field-theoretic formulation of composite fermions through a singular gauge transformation defined by

$$\Psi = \prod_{j < k} \left(\frac{z_j - z_k}{|z_j - z_k|} \right)^{2p} \Psi' \quad [35]$$

under which the eigenvalue problem of eqn [29] transforms into

$$H'\Psi' = E\Psi' \quad [36]$$

$$H' = \frac{1}{2m_b} \sum_i \left(p_i + \frac{e}{c} A(r_i) - \frac{e}{c} a(r_i) \right)^2 + V \quad [37]$$

$$a(r_i) = \frac{2p}{2\pi} \phi_0 \sum_j \nabla_i \phi_{ij} \quad [38]$$

where

$$\phi_{jk} = i \ln \frac{z_j - z_k}{|z_j - z_k|}$$

is the relative angle between the particles j and k . The magnetic field corresponding to $a(r_i)$ is given by

$$b_i = \nabla_i \times a(r_i) = 2p\phi_0 \sum_l \delta^2(r_i - r_l) \quad [39]$$

The above transformation thus amounts to attaching a point flux of strength $-2p\phi_0$ to each electron, which is how the composite fermion is modeled in this approach. (A flux quantum is topologically equivalent to a vortex.) This definition is reminiscent of the treatments of particles obeying fractional statistics (“anyons”) introduced by Leinaas and Myrheim (1977) and Wilczek (1982); an anyon is modeled as an electron bound to a point flux of magnitude $\alpha\phi_0$, where α determines the winding statistics.

It is not possible to proceed further without making approximations. The usual approach is to make a “mean-field” approximation, which amounts to spreading the point flux on each electron into a uniform magnetic field. Formally, one writes

$$A - a \equiv A^* + \delta A \quad [40]$$

$$\nabla \times A^* = B^* \hat{z} \quad [41]$$

The transformed Hamiltonian is written as

$$\begin{aligned} H' &= \frac{1}{2m_b} \sum_i \left(p_i + \frac{e}{c} A^*(r_i) \right)^2 + V + V' \\ &= H'_0 + V + V' \end{aligned} \quad [42]$$

V is the Coulomb interaction and V' denotes the terms containing δA . The solution to H'_0 is trivial, describing free fermions in an effective magnetic field B^* . We have thus decomposed the Hamiltonian into a part H'_0 , which can be solved exactly, and the rest, $V + V'$, which is to be treated perturbatively.

Lopez and Fradkin recast the problem in the language of functional integrals, which is suitable for studying corrections to the mean-field theory. One writes the zero-temperature quantum partition function

$$Z = \int \mathcal{D}\psi \mathcal{D}\psi^* \mathcal{D}a \exp \left(\frac{i}{\hbar} S \right) \quad [43]$$

$$S = \int d^2r \int dt \mathcal{L} \quad [44]$$

$$\begin{aligned} \mathcal{L} &= \psi^* (i\partial_t - a_0) \psi + \frac{1}{2m_b} \left| \left(-i\hbar\nabla + \frac{e}{c} A - \frac{e}{c} a \right) \psi \right|^2 \\ &\quad + \frac{1}{2p\phi_0} a_0 \nabla \times a + \int d^2r' \rho(r) V(r - r') \rho(r') \end{aligned} \quad [45]$$

where ψ and ψ^* are anticommuting Grassmann variables. The flux attachment is introduced through a Lagrange multiplier a_0 ; because a_0 enters linearly in the action, it can be integrated out to produce a delta function that imposes the constraint

$$\nabla \times a(r) = 2p\phi_0 \rho(r) = 2p\phi_0 \psi^*(r) \psi(r) \quad [46]$$

This formalism is closely related to the topological Chern–Simons (CS) field theory. Recall that the CS Lagrangian has the form

$$\mathcal{L}_{\text{CS}} \sim \epsilon^{\mu\nu\lambda} A_\mu F_{\nu\lambda} = 2\epsilon^{\mu\nu\lambda} A_\mu \partial_\nu A_\lambda \quad [47]$$

where $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$, and $\epsilon^{\mu\nu\lambda}$ is the antisymmetric Levy–Civita tensor, with $\epsilon^{012} = 1$. The index takes values $\mu=0,1,2$, the first being the time component and the remaining space components. The CS action is invariant, up to surface terms, under a gauge transformation, because the change in \mathcal{L}_{CS} under a functional variation $\delta A_\mu = \partial_\mu \Lambda$ is a total derivative.

Zhang *et al.* (1989) noted that the term proportional to $a_0 \nabla \times \mathbf{a}$ in eqn [45], which enforces flux attachment, is precisely equal to the CS Lagrangian in the Coulomb gauge. Write

$$\begin{aligned} \mathcal{L}_{\text{CS}} &= \frac{1}{4p\phi_0} \epsilon^{\mu\nu\lambda} a_\mu \partial_\nu a_\lambda \\ &= \frac{1}{2p\phi_0} \epsilon^{ij} a_0 \partial_i a_j - \frac{1}{4p\phi_0} \epsilon^{ij} a_i \partial_0 a_j \end{aligned} \quad [48]$$

where i, j represent the spatial components ($i, j=1,2$), and the time components have been displayed explicitly in the second step ($\partial_0 = \partial_t$). The first term on the right-hand side of eqn [48] is identical to the third term on the right-hand side of eqn [45]. In the Fourier space the last term is proportional to

$$\epsilon^{ij} a_i(\mathbf{q}, \omega) (-i\omega) a_j(-\mathbf{q}, -\omega) \quad [49]$$

By choosing the x -axis along \mathbf{q} , the Coulomb gauge condition $\mathbf{q} \cdot \mathbf{a} = 0$ implies $a_2(\mathbf{q}, \omega) = 0$, guaranteeing that the last term in eqn [48] is identically zero.

The constraint of eqn [46] is used to eliminate the two factors of density in the last term of eqn [45]. The action is then quadratic in the fermion field, which can be integrated out. Various response functions can be expressed as correlation functions of the vector potential field and their averages over the CS field configurations are evaluated perturbatively by standard diagrammatic methods.

The fermion CS theory is believed to capture the topological properties of composite fermions, but has not lent itself, because of the lack of a small parameter, to quantitative calculations. It is not known what classes of Feynman diagrams will need to be summed to eliminate the electron mass m_b (which is not a parameter of the lowest Landau problem – see eqn [30]) in the fermion CS

approach). Halperin *et al.* (1993) proceeded by replacing m_b by an adjustable parameter m^* , interpreted as the composite-fermion mass. Murthy and Shankar (1997) proposed to separate out the inter- and intra-Landau level degrees of freedom by making a sequence of further transformations.

Consequences

Fractional Quantum Hall Effect

The CF theory provides a simple understanding of why gaps open up at “fractional” fillings, which happens at those fillings $\nu = f$ for which composite fermions fill integral numbers of CF Landau levels. That results in Hall plateaus at $R_H = h/f e^2$ in the presence of disorder. The fractional QHE is thus understood as the integral QHE for composite fermions.

Sequences of Fractions

The integral fillings of composite fermions correspond to fractional fillings of electrons given by

$$\nu = \frac{|n|}{2p|n| \pm 1} \quad [50]$$

which are precisely the observed fractions. Some of these are:

$$f = \frac{|n|}{2|n| + 1} = \frac{1}{3}, \frac{2}{5}, \dots, \frac{10}{21} \quad [51]$$

$$f = \frac{|n|}{2|n| - 1} = \frac{2}{3}, \frac{3}{5}, \dots, \frac{10}{19} \quad [52]$$

$$f = \frac{|n|}{4|n| + 1} = \frac{1}{5}, \frac{2}{9}, \dots, \frac{6}{25} \quad [53]$$

$$f = \frac{|n|}{4|n| - 1} = \frac{2}{7}, \frac{2}{5}, \dots, \frac{6}{23} \quad [54]$$

Particle–hole symmetry in the lowest Landau level also implies fractions $1 - f$. The fractions appear in the form of sequences because they are all derived from the sequence of integers. The Hall quantization is exact because the right-hand side of eqn [50] is made up of whole numbers and therefore is not susceptible to small perturbations in the Hamiltonian. The CF theory unifies the FQHEs and IQHEs.

Fermi Sea at Half Filling

Equation [50] is consistent with the fact that only odd-denominator fractions have been observed in the lowest Landau level (i.e., with $f < 1$). Halperin *et al.* (1993) and Kalmeyer and Zhang (1992) proposed that at the simplest even-denominator fraction, namely $\nu = 1/2$, composite fermions form a Fermi sea. This was motivated by the fact that the effective magnetic field is $B^* = 0$ at $\nu = 1/2$. A number of experiments have directly measured the Fermi sea of composite fermions. The TSG effect with $f = 1/2$ is absent because the Fermi sea has gapless excitations.

Effective Magnetic Field

For small values of B^* (i.e., in the vicinity of $\nu = 1/2$), the cyclotron radius of composite fermions can be very large compared to the radius of the cyclotron orbit of a classical electron in B . Direct measurements of the cyclotron orbit in several geometric experiments have confirmed that the charge carriers experience a magnetic field B^* rather than B .

Fractional Charge

Laughlin (1983) showed that the presence of a gap at a fractional filling implies the existence of fractionally charged excitations. He obtained an excitation through the adiabatic insertion of a point flux quantum at, say the origin, which can be gauged away at the end leaving behind an exact excited state. The Faraday's law implies that the azimuthal component of the induced electric field is $E_\phi = -(2\pi r)^{-1} d\phi/dt$. The current density then is $j_r = \sigma_H E_\phi$, where $\sigma_H = fe^2/h$ is the Hall conductivity. The charge leaving the area defined by a circle of radius r per unit time is $2\pi r j_r$. The total charge leaving this area in the adiabatic process then is

$$Q = \int 2\pi r j_r dt = -\sigma_H \phi_0 = -fe \quad [55]$$

The charge excess associated with the excitation is therefore fe . It is in general not an elementary excitation. For $f = n/(2pn \pm 1)$, it can be shown to be a collection of n elementary excitations, giving a charge of $e^* = e/(2pn \pm 1)$ for a single elementary excitation.

Microscopic Tests

Exact solutions of the Schrödinger equation can be obtained, for a finite number of particles, by a brute-force diagonalization of the Hamiltonian in the

lowest LL subspace, which enables a rigorous and nontrivial testing of the CF theory. Figure 3 shows some typical comparisons, which help test both the qualitative and the quantitative aspects of the CF theory in a model-independent manner. The low-energy spectrum of interacting electrons at B is explicitly seen to have a one-to-one correspondence to that of weakly interacting electrons at B^* . Furthermore, there is a remarkably good quantitative agreement. The predicted energies agree with the exact energies to better than 0.05%, and the overlaps between the wave functions of eqn [31] with the exact eigenfunctions are close to 100%. Such comparisons are even more convincing in light of the fact that the wave functions of eqn [31] do not contain any adjustable parameters for the states at ν in eqn [50], because the ground state wave function and its low-energy excitations at $\nu^* = n$ are unique and fully known: the former is the Slater determinant corresponding to n filled

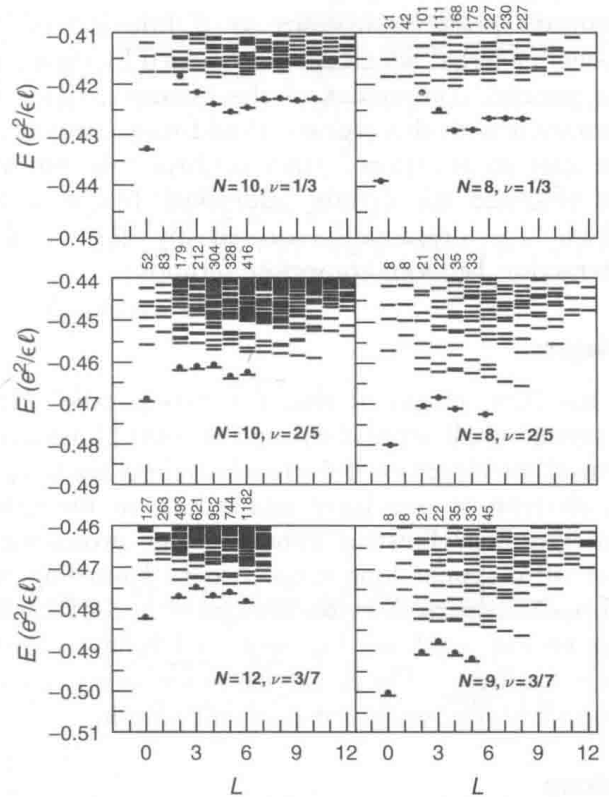


Figure 3 Exact spectra (dashes) for several particle numbers at $\nu = 1/3, 2/5$, and $3/7$. Dots show the CF prediction for the energy, obtained with no adjustable parameters. The electrons are taken to be confined on the surface of a sphere in the presence of a radial magnetic field; L is the total orbital angular momentum, and each dash represents a multiplet of $2L + 1$ degenerate states. The number on top is the dimension of the Fock space in the corresponding L sector. Reproduced from Jain JK (2000) The composite fermion: a quantum particle and its quantum fluids. *Physics Today* 39(4): 39–42, with permission from American Institute of Physics.

Landau levels, and the latter are the excitons. The predicted energies are calculated by determining the expectation values of the full Hamiltonian of eqn [30] with respect to the wave functions in eqn [31].

More Physics

Spin

At small Zeeman energies, partially spin-polarized or spin-unpolarized FQHE states become possible. The TSG effect with spin is well described by a generalization of the CF theory. The observed fractions are still given by eqn [50], but with

$$n = n_{\uparrow} + n_{\downarrow} \quad [56]$$

where n_{\uparrow} is the number of occupied spin-up Landau-like CF bands and n_{\downarrow} is the number of occupied spin-down Landau-like CF bands. There are in general several states with different spin polarizations possible at any given fraction. The observed quantum phase transitions as a function of the Zeeman energy, which can be changed by increasing the parallel component of the magnetic field, are consistent with this picture. Direct measurements of the spin polarization further confirm this, but also see evidence for certain additional fragile states, which are presumably caused by the residual interaction between composite fermions.

Bilayers

It has been proposed that for two parallel 2DES planes at small separations and at total filling $\nu=1$, neutral interlayer excitons (each exciton made up of an electron in one layer and a hole in the other) undergo Bose-Einstein condensation, producing a true off-diagonal long-range order. Tunneling and transport experiments by Eisenstein and collaborators provide evidence for nontrivial behavior under such conditions. The resistivity in the antisymmetric channel is very small but does not vanish.

Pairing

An even-denominator fraction $f=5/2$ has been observed. Writing $5/2=2+1/2$ and noting that the lowest LL contributes 2 (counting the spin degree of freedom), $\nu=5/2$ corresponds to a filling of $1/2$ in the second Landau level. The most promising scenario for the explanation of the $5/2$ effect is that composite fermions form a p -wave paired state, which opens up a gap to excitations. This state is believed to be well described by a

Pfaffian wave function proposed by Moore and Read (1991)

$$\Psi_{1/2}^{\text{Pf}} = \text{Pf} \left(\frac{1}{z_i - z_j} \right) \times \prod_{i < j} (z_i - z_j)^2 \exp \left(-\frac{1}{4} \sum_k |z_k|^2 \right) \quad [57]$$

The Pfaffian of an antisymmetric matrix M is defined, apart from an overall factor, as

$$\text{Pf}(M_{ij}) = A(M_{12}M_{34} \dots M_{N-1,N}) \quad [58]$$

where A is the antisymmetrization operator. The Bardeen-Cooper-Schrieffer wave function

$$\Psi_{\text{BCS}} = A[\phi_0(\mathbf{r}_1, \mathbf{r}_2)\phi_0(\mathbf{r}_3, \mathbf{r}_4) \dots \phi_0(\mathbf{r}_{N-1}, \mathbf{r}_N)] \quad [59]$$

has the same form as the Pfaffian in eqn [58]. Hence, $\text{Pf } 1/(z_i - z_j)$ describes a p -wave pairing of electrons, and $\Psi_{1/2}^{\text{Pf}}$ is interpreted as a paired state of composite fermions carrying two vortices.

FQHE of Composite Fermions

Recently, some fractions other than those in eqn [50] have been observed, for example, $f=4/11$ and $f=5/13$. These are understood as the delicate “fractional” QHE of composite fermions at $\nu^*=1+1/3$ and $\nu^*=1+2/3$.

TSG Effect in Higher Landau Levels

The short-range part of the Coulomb interaction is less effective in higher Landau levels because of the greater spread of the electron wave function. As a result, composite fermions are less stable, often losing to charge density wave states. A few fractions have been observed in the second Landau level ($1/3$, $2/3$, $2/5$, $1/2$) and one ($1/3$) in the third.

Edge states

There is a gap to excitations in the bulk at the magic fillings of eqn [50], but there is no gap at the edge of the sample. The dynamics of the low-energy edge excitations is formally equivalent to that of a chiral one-dimensional Tomonaga-Luttinger liquid. Wen (1991) argued that the exponent characterizing the long-distance behavior of this liquid is quantized, fully determined by the filling factor of the bulk state. Experimental studies of the tunneling of an external electron into the edge of an FQHE system provide evidence for a nontrivial

Tomonaga–Luttinger liquid but do not find the predicted universal value for the edge exponent.

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See also: Abelian Higgs Vortices; Aharonov–Bohm Effect; Chern–Simons Models: Rigorous Results; Fermionic Systems; Geometric Phases; Quantum Hall Effect; Quantum Phase Transitions; Quantum Statistical Mechanics: Overview.

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Free Interfaces and Free Discontinuities: Variational Problems

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Introduction

In several models coming from very different applications, one needs to describe physical phenomena where the state function may present some regions of discontinuity. We may think, for instance, of problems arising in fracture mechanics, where the function which describes the displacement of the body has a jump along the fracture, phase transitions, or also of problems of image reconstruction,

where the function that describes a picture (the intensity of black, e.g., in black-and-white pictures) has naturally some discontinuities along the profiles of the objects.

The Sobolev space analysis is then no longer appropriate for this kind of problem, since Sobolev functions cannot have jump discontinuities along hypersurfaces, as, on the contrary, is required by the models above. For a rigorous presentation of variational problems involving functions with discontinuities, the essential tool is the space, BV, of functions with bounded variation. The first ideas about this space were developed by De Giorgi in the 1950s, in order to provide a variational framework to

study the problems of minimal surfaces, and several monographs are now available on the subject. We quote, for instance, the classical volumes of Evans and Gariepy (1992), Federer (1969), Giusti (1984), Massari and Miranda (1984), Ziemer (1989), and the recent book by Ambrosio *et al.* (2000), where a systematic presentation is given, also in view of the applications mentioned above.

The Space BV

Consider a generic open subset Ω of \mathbb{R}^N , which, for simplicity, we take bounded and with a Lipschitz boundary. In the following, we denote by $\mathcal{L}^N(E)$, or simply $|E|$, the Lebesgue measure of E in \mathbb{R}^N , while \mathcal{H}^k denotes the k -dimensional Hausdorff measure.

Definition 1 We say that a function $u \in L^1(\Omega)$ is a function of bounded variation in Ω if its distributional gradient Du is an \mathbb{R}^N -valued finite Borel measure on Ω . In other words, we have

$$\int_{\Omega} u D_i \phi \, dx = - \int_{\Omega} \phi \, dD_i u \quad \forall \phi \in C_c^\infty(\Omega), \quad \forall i = 1, \dots, N \quad [1]$$

where $D_i u$ are finite Borel measures. The space of all functions of bounded variation in Ω is denoted by $BV(\Omega)$.

The space $BV(\Omega)$ is clearly a vector space and, with the norm

$$\|u\|_{BV(\Omega)} = \|u\|_{L^1(\Omega)} + |Du|(\Omega) \quad [2]$$

it becomes a Banach space. The total variation $|Du|(\Omega)$ appearing above is intended as

$$\begin{aligned} |Du|(\Omega) &= \sup \left\{ \sum_{i=1}^N \int_{\Omega} \phi_i \, dD_i u : \phi \in C_c^\infty(\Omega; \mathbb{R}^N), |\phi| \leq 1 \right\} \\ &= \sup \left\{ - \int_{\Omega} u \operatorname{div} \phi \, dx : \phi \in C_c^\infty(\Omega; \mathbb{R}^N), |\phi| \leq 1 \right\} \end{aligned}$$

and is sometimes indicated by $\int_{\Omega} |Du|$. The space $BV_{\text{loc}}(\Omega)$ is defined in a similar way, requiring that $u \in BV(\Omega')$ for every $\Omega' \subset\subset \Omega$.

From the point of view of functional analysis, the space $BV(\Omega)$ does not verify the nice properties of Sobolev spaces. In particular,

- the Banach space $BV(\Omega)$ is not separable;
- the Banach space $BV(\Omega)$ is not reflexive; and
- the class of smooth functions is not dense in $BV(\Omega)$ for the norm [2].

The above issues motivate why the norm [2] is not very helpful in the study of variational problems involving the space $BV(\Omega)$. On the contrary, the weak* convergence defined below is much more suitable to treat minimization problems for integral functionals.

Definition 2 We say that a sequence (u_n) weakly* converges in $BV(\Omega)$ to a function $u \in BV(\Omega)$ if $u_n \rightarrow u$ strongly in $L^1(\Omega)$ and $Du_n \rightarrow Du$ in the weak* convergence of measures.

The weak* convergence on $BV(\Omega)$ satisfies the following properties:

- *Compactness* Every bounded sequence in $BV(\Omega)$ for the norm [2] admits a weakly* convergent subsequence.
- *Lower-semicontinuity* The norm [2] is sequentially lower-semicontinuous with respect to the weak* convergence.
- *Density* Every function $u \in BV(\Omega)$ can be approximated, in the weak* convergence, by a sequence (u_n) of smooth functions.

The density property above can be actually made stronger: in fact, the approximation of (u_n) to u holds in the sense that

$$\begin{cases} u_n \rightarrow u \text{ strongly in } L^1(\Omega) \\ Du_n \rightarrow Du \text{ weakly* as measures} \\ |Du_n|(\Omega) \rightarrow |Du|(\Omega) \end{cases}$$

Further properties of the space $BV(\Omega)$ concern the embeddings into Lebesgue spaces, traces, and Poincaré-type inequalities. More precisely, we have:

- *Embeddings* The space $BV(\Omega)$ is embedded continuously into $L^{N/(N-1)}(\Omega)$ and compactly into $L^p(\Omega)$ for every $p < N/(N-1)$.
- *Traces* Every function $u \in BV(\Omega)$ has a boundary trace which belongs to $L^1(\partial\Omega)$, and the trace operator from $BV(\Omega)$ into $L^1(\partial\Omega)$ is continuous.
- *Poincaré inequalities* There exist suitable constants c_1 and c_2 such that for every $u \in BV(\Omega)$

$$\int_{\Omega} |u| \, dx \leq c_1 \left[|Du|(\Omega) + \int_{\partial\Omega} |u| \, d\mathcal{H}^{N-1} \right]$$

$$\int_{\Omega} |u - u_{\Omega}| \, dx \leq c_2 |Du|(\Omega)$$

$$\left(\text{where } u_{\Omega} = \frac{1}{|\Omega|} \int_{\Omega} u \, dx \right)$$

Sets of Finite Perimeter

An important class of functions with bounded variation are those that can be written as 1_E , the characteristic function of a set E , taking the value 1 on E and 0 elsewhere. This is the natural class where many phase-transition problems with sharp interfaces may be framed.

Definition 3 For a measurable set $E \subset \mathbb{R}^N$ the perimeter of E in Ω is defined as

$$\text{Per}(E, \Omega) = |D1_E|(\Omega)$$

The equality above is intended as $\text{Per}(E, \Omega) = +\infty$ whenever $1_E \notin \text{BV}(\Omega)$. If $\text{Per}(E, \Omega) < +\infty$ then the set E is called a set of finite perimeter in Ω .

Note that by the compactness property above for BV functions, a family of characteristic functions of sets with finite perimeter in a bounded open set Ω with equibounded perimeter is weakly*-precompact, and its limit is of the same form.

For a set E of finite perimeter in Ω , we may define the inner normal versor and the reduced boundary as follows.

Definition 4 Let E be a set of finite perimeter in Ω . We call reduced boundary ∂^*E the set of all points $x \in \Omega \cap \text{spt}|D1_E|$ such that the limit

$$\nu_E(x) = \lim_{r \rightarrow 0} \frac{D1_E(B_r(x))}{|D1_E|(B_r(x))}$$

exists and satisfies $|\nu_E(x)| = 1$. The vector $\nu_E(x)$ is called the generalized inner normal versor to E .

In order to link the measure-theoretical objects introduced above with some structure property of sets of finite perimeter, we introduce, for every $t \in [0, 1]$ and every measurable set $E \subset \mathbb{R}^N$, the set E^t defined by

$$E^t = \left\{ x \in \mathbb{R}^N : \lim_{r \rightarrow 0} \frac{|E \cap B_r(x)|}{|B_r(x)|} = t \right\} \quad [3]$$

For instance, if E is a smooth domain of \mathbb{R}^N , E^1 is the interior part of E , E^0 is its exterior part, while $E^{1/2}$ is the boundary ∂E .

The main properties of the reduced boundary and of the generalized inner normal versor are stated in the following result.

Theorem 5 Let E be a set of finite perimeter in Ω . Then its reduced boundary ∂^*E coincides \mathcal{H}^{N-1} -a.e. with the set $E^{1/2}$ introduced in Definition 3, and we have the equality

$$\text{Per}(E, \Omega) = \mathcal{H}^{N-1}(\Omega \cap \partial^*E) = \mathcal{H}^{N-1}(\Omega \cap E^{1/2})$$

Moreover, the generalized inner normal versor $\nu_E(x)$ exists for \mathcal{H}^{N-1} -a.e. $x \in \partial^*E$, and we have

$$D1_E = \nu_E(x) \mathcal{H}^{N-1} \llcorner \partial^*E$$

Note that the lower-semicontinuity of $|D1_E|(\Omega)$ entails the lower-semicontinuity of $E \mapsto \mathcal{H}^{N-1}(\Omega \cap \partial^*E)$ with respect to the weak*-convergence of 1_E . As a consequence, we may apply the direct methods of the calculus of variations to obtain, for example, existence of minimizers of

$$\min \left\{ \text{Per}(E, \mathbb{R}^N) - \int_E g \, dx \right\}$$

that are sets with prescribed mean curvature g . This lower-semicontinuity property can be further generalized, for example, as in the following result for anisotropic perimeters.

Theorem 6 Let $\varphi: S^{N-1} \rightarrow \mathbb{R}$ be a Borel function. The energy

$$\int_{\Omega \cap \partial^*E} \varphi(\nu_E) \, d\mathcal{H}^{N-1}$$

is lower-semicontinuous with respect to the weak*-convergence of 1_E in $\text{BV}(\Omega)$ if and only if the positively one-homogeneous extension of φ from S^{N-1} to \mathbb{R}^N is convex.

This result immediately implies the existence of solutions of isovolumetric problems of the form

$$\min \left\{ \int_{\partial^*E} \varphi(\nu_E) \, d\mathcal{H}^{N-1} : |E| = c \right\}$$

whose solutions are obtained by suitably scaling the Wulff shape of φ .

The Structure of BV Functions

The simplest situation occurs when $N = 1$ and so Ω is an interval of the real line. In this case, decomposing the derivative u' into positive and negative parts, and taking their primitives, we obtain that $u \in \text{BV}(\Omega)$ if and only if u is the sum of two bounded monotone functions (one increasing and one decreasing). Therefore, in the one-dimensional case, the BV functions share all the properties of monotone functions.

The situation is more delicate when $N > 1$, for which we need the notion of approximate limit.

Definition 7 Let $u \in \text{BV}(\Omega)$. We say that u has the approximate limit z at x if

$$\lim_{r \rightarrow 0} \frac{1}{|B_r(x)|} \int_{B_r(x)} |u(y) - z| \, dy = 0$$

The set where no approximate limit exists is called the approximate discontinuity set, and is denoted by S_u . In a similar way, when $x \in S_u$ we may define the approximate values z^+ and z^- , by requiring that

$$\lim_{r \rightarrow 0} \frac{1}{|B_r^+(x, \nu)|} \int_{B_r^+(x, \nu)} |u(y) - z^+| dy = 0$$

$$\lim_{r \rightarrow 0} \frac{1}{|B_r^-(x, \nu)|} \int_{B_r^-(x, \nu)} |u(y) - z^-| dy = 0$$

where

$$B_r^+(x, \nu) = \{y \in B_r(x): (y - x) \cdot \nu > 0\}$$

$$B_r^-(x, \nu) = \{y \in B_r(x): (y - x) \cdot \nu < 0\}$$

Analogous definitions can be given in the vector-valued case, when $u \in BV(\Omega; \mathbb{R}^m)$.

The triplet (z^+, z^-, ν) in Definition 7 is unique up to interchanging z^+ with z^- and changing sign to ν , and is denoted by $(u^+(x), u^-(x), \nu_u(x))$.

We are now in a position to describe the structure of the measure Du when $u \in BV(\Omega)$, or more generally $u \in BV(\Omega; \mathbb{R}^m)$. We first apply the Radon–Nikodym theorem to Du and we decompose it into absolutely continuous and singular parts: $Du = (Du)^a + (Du)^s$. We denote by ∇u the density of the absolutely continuous part, so that we have

$$Du = \nabla u \cdot \mathcal{L}^N + (Du)^s$$

The singular part $(Du)^s$ can be further decomposed into an $(N - 1)$ -dimensional part, concentrated on the approximate discontinuity set S_u , and the remaining part, which vanishes on all sets with finite \mathcal{H}^{N-1} measure. More precisely, if $u \in BV(\Omega; \mathbb{R}^m)$, we have

$$Du = \nabla u \cdot \mathcal{L}^N + (u^+(x) - u^-(x)) \otimes \nu_u(x) \cdot \mathcal{H}^{N-1} \llcorner S_u + (Du)^c \quad [4]$$

the three terms on the right-hand side are mutually singular and are, respectively, called the absolutely continuous part, the jump part, and the Cantor part of the gradient measure Du .

In the vector-valued case, Du is an $m \times N$ matrix of finite Borel measures, ∇u is an $m \times N$ matrix of functions in $L^1(\Omega)$, and the jump term in [4] is an $(N - 1)$ -dimensional measure of rank 1. The structure of the Cantor part $(Du)^c$ is described by the Alberti's rank-1 theorem (see Alberti (1993)).

Theorem 8 For every $u \in BV(\Omega; \mathbb{R}^m)$ the Cantor part $(Du)^c$ is a measure with values in the $m \times N$ matrices of rank 1.

Convex Functionals on BV

Many problems of the calculus of variations deal with the minimization of energies of the form

$$F(u) = \int_{\Omega} f(x, u, Du) dx \quad [5]$$

The direct methods to obtain the existence of at least a minimizer require some coercivity hypotheses on F , as well as its lower-semicontinuity. This last issue, already rather delicate when working in Sobolev spaces (see, e.g., Buttazzo (1989) and Dacorogna (1989)), presents additional difficulties when the unknown function u varies in the space $BV(\Omega)$, due to the fact that Du is a measure, and the precise meaning of the integral in [5] has to be clarified.

In this section, we limit ourselves to consider the simpler situation of convex functionals, and we also assume that the integrand $f(x, u, Du)$ depends only on x and Du . It is then convenient to study the problem in the framework of functionals defined on the space of finite Borel vector measures $\mathcal{M}(\Omega; \mathbb{R}^k)$. Let $f: \mathbb{R}^N \times \mathbb{R}^k \rightarrow [0, +\infty]$ be a Borel function such that

- f is lower-semicontinuous, and
- $f(x, \cdot)$ is convex for every $x \in \mathbb{R}^N$.

We denote by $f^\infty(x, z)$ the recession function associated with f , given by

$$f^\infty(x, z) = \lim_{t \rightarrow +\infty} \frac{f(x, z_0 + tz)}{t}$$

where z_0 is any point in \mathbb{R}^k such that $f(x, z_0) < +\infty$ (in fact, the definition above is independent of the choice of z_0). Then we may consider the functional

$$F(\lambda) = \int_{\Omega} f(x, \lambda^a(x)) dx + \int_{\Omega} f^\infty\left(x, \frac{d\lambda^s}{d|\lambda^s|}\right) d|\lambda^s| \quad [6]$$

where $\lambda = \lambda^a \cdot dx + \lambda^s$ is the Lebesgue–Nikodym decomposition of λ into absolutely continuous and singular parts, and the notation $d\lambda^s/d|\lambda^s|$ stands for the density of λ^s with respect to its total variation $|\lambda^s|$. For simplicity, the last term on the right-hand side of [6] is often denoted by $\int_{\Omega} f^\infty(x, \lambda^s)$.

For the functional F , the following lower-semicontinuity result holds (see, e.g., Buttazzo (1989)).

Theorem 9 Under the assumptions above the functional [6] is sequentially lower-semicontinuous for the weak* convergence on $\mathcal{M}(\Omega; \mathbb{R}^k)$. Moreover, if

$$f(x, z) \geq c_0|z| - a(x)$$

with $c_0 > 0$ and $a \in L^1(\Omega)$ [7]

then the functional F turns out to be coercive for the same topology.

From Theorem 9 we deduce immediately a lower-semicontinuity result for functionals defined on $BV(\Omega; \mathbb{R}^m)$.

Corollary 10 *Under the assumptions above on the integrand f (with $k = mN$) the functional defined on $BV(\Omega; \mathbb{R}^m)$ by*

$$F(u) = \int_{\Omega} f(x, (Du)^a) dx + \int_{\Omega} f^{\infty}\left(x, \frac{d(Du)^s}{d|Du|^s}\right) d|Du|^s \quad [8]$$

is sequentially lower-semicontinuous for the weak* convergence. Moreover, under the assumption [7] the functional F is coercive with respect to the same topology.

For some extensions of the result above to the case when $f(x, \cdot)$ is quasiconvex (in the vector-valued situation $m > 1$), we refer the interested reader to Fonseca and Müller (1992) and references therein.

Fixing boundary data is another difference between variational problems on Sobolev spaces and on BV spaces. Due to the fact that the class $\{u \in BV(\Omega): u = u_0 \text{ on } \partial\Omega\}$ is not weakly* closed, to set in a correct way a minimum problem of Dirichlet type on $BV(\Omega)$ with datum $u_0 \in BV(\mathbb{R}^N)$ it is convenient to consider a larger domain $\Omega' \supset \supset \Omega$ and for every $u \in BV(\Omega)$ the extended function

$$\tilde{u} = \begin{cases} u & \text{on } \Omega \\ u_0 & \text{on } \Omega' \setminus \Omega \end{cases}$$

whose distributional gradient is

$$D\tilde{u} = Du \llcorner \Omega + Du_0 \llcorner \Omega' \setminus \bar{\Omega} + (u_0 - u)\nu_{\Omega} \mathcal{H}^{N-1} \llcorner \partial\Omega$$

ν_{Ω} being the exterior normal vector to Ω . We have then the following functional on $BV(\Omega')$:

$$\begin{aligned} \tilde{F}(\tilde{u}) &= \int_{\Omega'} f(x, (D\tilde{u})^a) dx + \int_{\Omega'} f^{\infty}(x, (D\tilde{u})^s) \\ &= \int_{\Omega} f(x, (Du)^a) dx + \int_{\Omega' \setminus \Omega} f(x, (Du_0)^a) dx \\ &\quad + \int_{\Omega} f^{\infty}(x, (Du)^s) + \int_{\Omega' \setminus \bar{\Omega}} f^{\infty}(x, (Du_0)^s) \\ &\quad + \int_{\partial\Omega} f^{\infty}(x, (u_0 - u)\nu_{\Omega}) d\mathcal{H}^{N-1} \end{aligned}$$

If we drop the constant term

$$\int_{\Omega' \setminus \Omega} f(x, (Du_0)^a) dx + \int_{\Omega' \setminus \bar{\Omega}} f^{\infty}(x, (Du_0)^s)$$

irrelevant for the minimization, we end up with the functional

$$F_{u_0}(u) = F(u) + \int_{\partial\Omega} f^{\infty}(x, (u_0 - u)\nu_{\Omega}) d\mathcal{H}^{N-1}$$

where F is as in [8]. The Dirichlet problem we consider is then

$$\min \left\{ F(u) + \int_{\partial\Omega} f^{\infty}(x, (u_0 - u)\nu_{\Omega}) d\mathcal{H}^{N-1}; \right. \\ \left. u \in BV(\Omega) \right\} \quad [9]$$

For instance, if $f(z) = |z|$, problem [9] becomes

$$\min \left\{ \int_{\Omega} |Du| + \int_{\partial\Omega} |u - u_0| d\mathcal{H}^{N-1}; u \in BV(\Omega) \right\}$$

Under the assumptions considered, the problem above admits a solution $u \in BV(\Omega)$, but in general we do not have $u = u_0$ on $\partial\Omega$ in the sense of BV traces.

Nonconvex Functionals on BV

In order to introduce the class of nonconvex functionals on $BV(\Omega)$, let us denote $v = Du$ so that every functional $\Phi(v)$ provides an energy $F(u)$. If we work in the setting of Sobolev spaces, we have $u \in W^{1,p}(\Omega)$ ($p \geq 1$), which implies $v \in L^p(\Omega; \mathbb{R}^N)$; now, it happens that in this case all “interesting” functionals Φ are convex. More precisely, it can be proved that a functional $\Phi: L^p(\Omega; \mathbb{R}^N) \rightarrow [0, +\infty]$, which is

- sequentially lower-semicontinuous for the weak convergence of $L^p(\Omega; \mathbb{R}^N)$, and
- local on $L^p(\Omega; \mathbb{R}^N)$ in the sense that $\Phi(v + w) = \Phi(v) + \Phi(w)$ whenever $v \cdot w \equiv 0$ in Ω ,

has to be necessarily convex, and of the form

$$\Phi(v) = \int_{\Omega} \phi(x, v(x)) dx$$

for a suitable integrand ϕ such that $\phi(x, \cdot)$ is convex. Then the energies $F(u)$ defined on Sobolev spaces and obtained by a functional $\Phi(v)$ through the identification $v = Du$ are necessarily convex. This is no longer true if Φ is defined on the space $\mathcal{M}(\Omega; \mathbb{R}^N)$ of measures, and hence F is defined on $BV(\Omega)$. The first example of a nonconvex functional Φ on $\mathcal{M}(\Omega; \mathbb{R}^N)$ in the literature comes from the so-called Mumford-Shah model for computer vision (see below) and is given by

$$\Phi(\lambda) = \int_{\Omega} |\lambda^a(x)|^2 dx + \#(A_{\lambda})$$

where λ^a is the absolutely continuous part of λ , A_λ is the set of atoms of λ , and $\#$ is the counting measure. The functional Φ is set equal to $+\infty$ on all measures λ whose singular part λ^s is nonatomic. A general representation result (see Bouchitte and Buttazzo (1992) and references therein) establishes that a functional $\Phi: \mathcal{M}(\Omega; \mathbb{R}^N) \rightarrow [0, +\infty]$, which is

- sequentially lower-semicontinuous for the weak* convergence of $\mathcal{M}(\Omega; \mathbb{R}^N)$, and
- local on $\mathcal{M}(\Omega; \mathbb{R}^N)$ in the sense that $\Phi(\lambda + \nu) = \Phi(\lambda) + \Phi(\nu)$ whenever λ and ν are mutually singular in Ω ,

has to be of the form

$$\Phi(\lambda) = \int_{\Omega} \phi(x, \lambda^a) d\mu + \int_{\Omega} \phi^\infty(x, \lambda^c) + \int_{\Omega} \psi(x, \lambda^\#(x)) d\#$$

where μ is a non-negative measure, $\lambda = \lambda^a \cdot dx + \lambda^c + \lambda^\#$ is the decomposition of λ into absolutely continuous, Cantor, and atomic parts, $\phi(x, v)$ is an integrand convex in v , and ϕ^∞ is its recession function. The novelty is now represented by the integrand $\psi(x, v)$ which has to be subadditive in v and satisfying the compatibility condition

$$\lim_{t \rightarrow +\infty} \frac{\phi(x, tv)}{t} = \lim_{t \rightarrow 0^+} \frac{\psi(x, tv)}{t}$$

When ϕ has a superlinear growth the condition above gives that the slope of $\psi(x, \cdot)$ at the origin has to be infinite. For instance, in the Mumford–Shah case we have

$$\phi(x, v) = |v|^2, \quad \psi(x, v) = \begin{cases} 1 & \text{if } v \neq 0 \\ 0 & \text{if } v = 0 \end{cases} \quad [10]$$

Coming back to the case $u \in \text{BV}(\Omega)$, we have the decomposition (see [4]):

$$Du = \nabla u \cdot \mathcal{L}^N + (Du)^c + [u] \nu_u(x) \cdot \mathcal{H}^{N-1} \llcorner S_u$$

where we considered, for simplicity, only the scalar case $m=1$ and denoted by $[u]$ the jump $u^+ - u^-$. We have then the functional

$$F(u) = \int_{\Omega} \phi(x, \nabla u) dx + \int_{\Omega} \phi^\infty(x, (Du)^c) + \int_{S_u} \psi(x, [u] \nu_u) d\mathcal{H}^{N-1}$$

For instance, in the homogeneous–isotropic case, when $\phi(x, v)$ and $\psi(x, v)$ are independent

of x and depend only on $|v|$, the formula above reduces to

$$F(u) = \int_{\Omega} \phi(|\nabla u|) dx + \beta |Du|^c(\Omega) + \int_{S_u} \psi(|[u]|) d\mathcal{H}^{N-1} \quad [11]$$

where β, ϕ, ψ satisfy the compatibility condition

$$\beta = \phi^\infty(1) = \lim_{t \rightarrow 0^+} \frac{\psi(t)}{t} \quad [12]$$

In the original Mumford–Shah model for computer vision, Ω is a rectangle of the plane, $u_0: \Omega \rightarrow [0, 1]$ represents the gray level of a picture, c_1 and c_2 are positive scale and contrast parameters, and the variational problem under consideration is

$$\min \left\{ \int_{\Omega} |\nabla u|^2 dx + c_1 \int_{\Omega} |u - u_0|^2 dx + c_2 \mathcal{H}^{N-1}(S_u) : (Du)^c \equiv 0 \right\} \quad [13]$$

The solution u then represents the reconstructed image, whose contours are given by the jump set S_u . We refer to Giorgi and Ambrosio (1988) and to the book by Morel and Solimini (1995) for further details about this model.

Analogously, in the case of the study of fractures of an elastic membrane, a problem similar to [13] provides the vertical displacement u of the membrane, together with its fracture set S_u . We refer to some recent papers (see Dal Maso and Toader (2002) and Francfort and Marigo (1998), and references therein) for a more detailed description of fracture mechanics problems, even in the more delicate vectorial setting of elasticity.

Using the functional F in [11] we have the generalized Mumford–Shah problem,

$$\min \left\{ F(u) + c_1 \int_{\Omega} |u - u_0|^2 dx : u \in \text{BV}(\Omega) \right\}$$

where ϕ is convex, ψ is subadditive, and the compatibility condition [12] is fulfilled.

If we set $K = S_u$ and assume that it is closed, the Mumford–Shah problem can be rewritten as

$$\min \left\{ \int_{\Omega \setminus K} |\nabla u|^2 dx + c_1 \int_{\Omega \setminus K} |u - u_0|^2 dx + c_2 \mathcal{H}^{N-1}(K \cap \Omega) : K \subset \bar{\Omega} \text{ closed}, \right. \\ \left. u \in H^1(\Omega \setminus K) \right\}$$

and this justifies the name “free discontinuity problems,” which is often used in this setting.

The regularity properties of optimal pairs (u, K) are far from being fully understood; some partial results are available but the Mumford–Shah conjecture:

- in the case $N=2$ for an optimal pair (u, K) the set K is locally the finite union of $C^{1,1}$ arcs

remains still open. We refer to Ambrosio *et al.* (2000) for a list of the regularity results on the problem above that are known thus far.

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Free Probability Theory

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Introduction

Free probability is a probability theory adapted to quantities with the highest degree of noncommutativity. A basic feature of this is that the definition of independence is modified in such a way that the freely independent random variables will not commute in general. The exploration of this notion of independence, which was initially motivated by questions about operator algebras (Voiculescu 1985), has produced a theory that runs parallel to an unexpectedly large part of classical probability theory. The applications of the theory have also gone into unexpected directions, once it turned out that the large- N limit of systems of random matrices is a key asymptotic model in the theory (Voiculescu 1991). There are several signs like the connections to large N for random matrices and to the combinatorics of noncrossing partitions (Speicher 1998) (which correspond to certain planar diagrams), that perhaps these

connections may go even further towards the large- N limit of models in gauge theory.

In this article the noncommutative probability and the random matrix angle will be emphasized and very little will be said about the operator algebras and the combinatorics. After discussing free independence and models based on free products of groups and creation and annihilation operators on the Boltzmann full Fock space, we continue with the semicircle law, which is the substitute for the Gauss law in this context, and with the nonlinear free harmonic analysis arising from addition and multiplication of free random variables.

We then devote two longer sections to the asymptotic free independence of large random matrices and to free entropy, the free probability analog of Shannon's information-theoretic entropy for continuous random variables.

Freeness of Noncommutative Random Variables

Classical probability deals with expectation values of numerical random variables, that is, with

numerical functions on a space of events and with their integrals with respect to a probability measure on the space of events. In noncommutative probability, the random variables, like quantum-mechanical quantities, are elements of a noncommutative algebra A over \mathbb{C} , with unit $1 \in A$, which is endowed with a linear expectation functional $\varphi: A \rightarrow \mathbb{C}$, so that $\varphi(1) = 1$. Frequently, A is a $*$ -algebra of operators on some Hilbert space \mathcal{H} and $\varphi(T) = \langle T\xi, \xi \rangle$ for some unit vector $\xi \in \mathcal{H}$. We call (A, φ) a noncommutative probability space and the elements $a \in A$, noncommutative random variables. In this section we shall discuss the basics around the notion of freeness (Voiculescu 1985), which plays the role of independence in free probability.

If $\alpha = (a_i)_{i \in I} \subset A$ is a family of noncommutative random variables, the role of joint distribution is played by the collection of noncommutative moments $\varphi(a_{i_1} \dots a_{i_n})$. This can also be extended by linearity to a distribution functional $\Phi_\alpha: \mathbb{C}\langle X_i | i \in I \rangle \rightarrow \mathbb{C}$, where $\mathbb{C}\langle X_i | i \in I \rangle$ is the ring of polynomials in noncommutative indeterminates $X_i (i \in I)$ and

$$\Phi_\alpha(P(X_i | i \in I)) = \varphi(P(a_i | i \in I))$$

If A is a C^* -algebra of operators on \mathcal{H} , $a = a^* \in A$ and $\varphi(\cdot) = \langle \cdot \xi, \xi \rangle$, the distribution of a can also be identified with the probability measure μ_a on \mathbb{R}

$$\mu_a(\omega) = \langle E(\omega; a) \xi, \xi \rangle$$

where $E(\cdot; a)$ is the spectral measure of a . Indeed, then

$$\Phi_a(P(X)) = \int P(t) d\mu_a(t)$$

A family $(A_i)_{i \in I} \subset A, 1 \in A_i$ of subalgebras is “free” (which is short for freely independent) if

$$\varphi(a_1 \dots a_n) = 0$$

whenever $a_j \in A_{i_j}, 1 \leq j \leq n, i_j \neq i_{j+1}$ and $\varphi(a_j) = 0$. (Here it is only required that consecutive a_j ’s be in different A_i ’s. Thus, we may have $i_1 = i_3$, provided $i_1 \neq i_2$.)

A family of sets of random variables $(\omega_i)_{i \in I}, \omega_i \subset A$ is free if the algebras A_i generated by $1 \cup \{\omega_i\}$ are free in (A, φ) .

Except for rather trivial situations, free random variables in (A, φ) do not commute.

Note also that, as in the case of classical independence, if $(\omega_i)_{i \in I}$ are disjoint freely independent sets of random variables, then, if the distributions $\Phi_{\omega_i} (i \in I)$ are given, the distribution Φ_ω of $\omega = \bigcup_{i \in I} \omega_i$ is completely determined.

Example 1 Let the group G be the free product of its subgroups $(G_i)_{i \in I}$, that is, G is generated by these

subgroups and there is no nontrivial relation among elements of different G_i ’s. Further, let λ be the regular representation $\lambda(g)e_h = e_{gh}$ of G on the Hilbert space with orthonormal basis $(e_g)_{g \in G}$. Then, with respect to the expectation functional $\tau(T) = \langle Te_e, e_e \rangle$ on operators on $\ell^2(G)$, the sets $(\lambda(G_i))_{i \in I}$ are freely independent.

Example 2 If \mathcal{H} is a complex Hilbert, let $\mathcal{TH} = \bigoplus_{k \geq 0} \mathcal{H}^{\otimes k}$ denote the full Boltzmann Fock space, with vacuum vector 1 so that $\mathcal{H}^{\otimes 0} = \mathbb{C}1$. If $h \in \mathcal{H}$ and $\xi \in \mathcal{TH}$, let $l(h)\xi = h \otimes \xi$ denote the left creation operator and $\varphi(X) = \langle X1, 1 \rangle$ the vacuum expectation. Then, if the $\mathcal{H}_i (i \in I)$ are pairwise orthogonal subspaces in \mathcal{H} , the $*$ -subalgebras of operators generated by $l(\mathcal{H}_i) \cup l^*(\mathcal{H}_i)$, indexed by $i \in I$, are freely independent with respect to φ .

Free Independence with Amalgamation over a Subalgebra

The classical notion of conditional independence also has a free counterpart based on the notion of free independence with amalgamation over a subalgebra. This subject is technically more complicated and we will only aim at giving an idea about what kind of concepts are involved.

In the classical context, if (X, Σ, μ) is a probability space with a σ -algebra Σ , then the conditional independence with respect to a σ -subalgebra of events, $\Sigma_0 \subset \Sigma$, amounts to replacing in the definition of independence the expectation functional (which is the integral with respect to μ) by the conditional expectation functional $L^\infty(X, \Sigma, \mu) \xrightarrow{E} L^\infty(X, \Sigma_0, \mu(\Sigma_0))$.

In free probability, one considers an extension of the theory, from the (A, φ) framework to an (A, Φ, B) framework (Voiculescu 1995), where A is an algebra with unit over \mathbb{C} , $B \ni 1$ is a subalgebra, and $\Phi: A \rightarrow B$ is B - B -bilinear and $\Phi|_B = \text{id}_B$. Then the definition of B -freeness (or free independence with amalgamation over B) of a family of subalgebras $(A_i)_{i \in I}, B \subset A_i \subset A$ requires that

$$\Phi(a_1 \dots a_n) = 0$$

whenever $a_j \in A_{i_j}, i_j \neq i_{j+1} (1 \leq j \leq n)$, and $\Phi(a_j) = 0$.

In the case of a unital $*$ -algebra of bounded operators M with an expectation functional $\tau(\cdot) = \langle \cdot \xi, \xi \rangle$ which is tracial (i.e., $\tau([m_1, m_2]) = 0$ if $m_1, m_2 \in M$) and given a subalgebra $1 \in N \subset M$, as in the classical theory, there is a certain canonical construction in operator algebra theory of a “conditional expectation” $\Phi: \bar{M} \rightarrow \bar{N}$, where \bar{M}, \bar{N} are

algebras of operators obtained as completion-separates from M and N . With this construction, in the trace-state setting there is complete analogy with the classical notion of conditional independence.

Several other constructions of free probability have been extended to the (A, Φ, B) B -valued context.

A group-theoretic example similar to Example 1 can be constructed from a group G which is a free product with amalgamation over a subgroup $H \subset G$ of subgroups $H \subset G_i \subset G_i \in I$. Then A is the algebra constructed from the left-regular representation of G , whereas B is an algebra constructed from the left-regular representation of H .

The Semicircle Law

In free probability the semicircle law appears as the limit law in the free central limit theorem (Voiculescu 1985). Here is a weak, rather algebraic, version of this fact:

If $(a_n)_{n \in \mathbb{N}}$ are freely independent in (A, φ) and satisfy the conditions that

$$\begin{aligned}\varphi(a_n) &= 0 (n \in \mathbb{N}) \\ \lim_{N \rightarrow \infty} N^{-1} \sum_{1 \leq n \leq N} \varphi(a_n^2) &= 1 \\ \sup_{n \in \mathbb{N}} |\varphi(a_n^k)| &= C_k < \infty (k \in \mathbb{N})\end{aligned}$$

then, if $S_N = N^{-1/2} \sum_{1 \leq n \leq N} a_n$, we have the convergence of moments of the distribution of S_N to the semicircle distribution

$$\lim_{N \rightarrow \infty} \varphi(S_N^k) = (2\sigma)^{-1} \int_{-2}^2 t^k (4 - t^2)^{1/2} dt$$

Thus, the semicircle law, given by the density $(2\pi)^{-1} (4 - t^2)^{1/2}$ on $[-2, 2]$ is the free analog of the $(0, 1)$ Gauss law.

Two coincidences involving the semicircle law should be noted.

The field operators $s(h) = 2^{-1}(l(h) + l(h)^*)$ on the Boltzmann Fock space (Example 2) have semicircle distributions with respect to the vacuum expectation $\epsilon(\cdot) = \langle \cdot, 1 \rangle$. It turns out that this goes farther: if $\mathcal{H} = \mathcal{H}_{\mathbb{R}} \otimes_{\mathbb{R}} \mathbb{C}$ is the complexification of a real Hilbert space, then the map $\mathcal{H}_{\mathbb{R}} \ni h \rightarrow s(h)$ is the analog in free probability of the Gaussian process over the Hilbert space $\mathcal{H}_{\mathbb{R}}$ (Voiculescu 1985). It is often called the semicircular process over $\mathcal{H}_{\mathbb{R}}$. This points to an important connection of free probability to the full Boltzmann statistics.

The other coincidence is that the semicircle law is well known as the Wigner limit distribution of

eigenvalues of large Gaussian random matrices. As we shall see, this is a clue to a deep connection of free probability to the large- N limit of random matrices (Voiculescu 1991).

Free Convolution Operations

In classical probability theory, the distribution of the sum of two independent random variables is computed by the convolution product of their distributions. This has a free probability analog. If a, b are free random variables in (A, φ) with distributions $\mu_a, \mu_b : \mathbb{C}[X] \rightarrow \mathbb{C}$, then the joint distribution $\mu_{\{a, b\}}$ is completely determined by μ_a, μ_b and in particular μ_{a+b} , the distribution of $a + b$, also depends only on μ_a, μ_b . It follows that there is an additive free convolution operation \boxplus on distributions so that $\mu_a \boxplus \mu_b = \mu_{a+b}$ whenever a, b are free (Voiculescu 1985). The same can be done with multiplication replacing addition, and this defines the multiplicative free convolution operation \boxtimes by the equation $\mu_a \boxtimes \mu_b = \mu_{ab}$, when a, b are free (Voiculescu 1985). A slightly surprising feature of \boxtimes is that in spite of noncommutativity of a and b , the multiplicative operation \boxtimes turns out to be commutative, which of course is obvious for \boxplus .

In the classical context, convolutions are bilinear operations which can be computed using integrals. The free convolutions are quite nonlinear and their computation is via another route, which can also be explained by a classical analogy. Classically, the logarithm of the Fourier transform linearizes convolution, that is,

$$\log \mathcal{F}(\mu * \nu) = \log \mathcal{F}(\mu) + \log \mathcal{F}(\nu)$$

and we may compute $\mu * \nu$ as the $(\log \mathcal{F})^{-1}$ of $\log \mathcal{F}(\mu) + \log \mathcal{F}(\nu)$. The linearizing transform for \boxplus is the R -transform (Voiculescu 1986), which is obtained by the following procedure.

If $\mu : \mathbb{C}[X] \rightarrow \mathbb{C}$ is a distribution, let $G_{\mu}(z) = z^{-1} + \sum_{n \geq 1} \mu(X^n) z^{-n-1}$, which, in case μ is a compactly supported probability measure on \mathbb{R} , is the Laurent series at ∞ of the Cauchy transform

$$\int \frac{d\mu(t)}{t - z}$$

From this, one obtains, by inversion at ∞ , the series K_{μ} , so that $G_{\mu}(K_{\mu}(z)) = z$ and one defines $R_{\mu}(z) = K_{\mu}(z) - z^{-1}$, which is a power series in z . Then

$$R_{\mu \boxplus \nu} = R_{\mu} + R_{\nu}$$

In case the distribution corresponds to a measure, the formal inversion amounts to inverting an analytic function.

For the multiplicative operation \boxplus , it is more convenient to describe an analog of the Mellin transform, that is, no logarithm will be taken. This is the S -transform (Voiculescu 1991), obtained as follows.

If $\mu: \mathbb{C}[X] \rightarrow \mathbb{C}$ is a distribution with $\mu(X) \neq 0$, one forms $\psi_\mu(z) = \sum_{n \geq 1} \mu(X^n) z^n$ and its inverse χ_μ so that $\psi_\mu(\chi_\mu(z)) = z$. Then

$$S_\mu(z) = z^{-1}(1+z)\chi_\mu(z)$$

has the property that

$$S_{\mu \boxplus \nu} = S_\mu S_\nu$$

The free central limit theorem can be easily proved using the R -transform. Another easy application of the R -transform is to find the free analog of the Poisson law, that is,

$$\lim_{n \rightarrow \infty} ((1-a/n)\delta_0 + a/n\delta_1)^{\boxplus}$$

where $a > 0$. The free Poisson law is

$$\mu = \begin{cases} (1-a)\delta_0 + \nu & \text{if } 0 \leq a \leq 1 \\ \nu & \text{if } a > 1 \end{cases}$$

where ν has support $[(1-a^{1/2})^2, (1+a^{1/2})^2]$ and density $(2\pi t)^{-1}(4a - (t - (1+a))^2)^{1/2}$. This distribution is well known in random matrix theory as the Marchenko–Pastur distribution, again a coincidence pointing to a random matrix theory connection.

Because probability measures on \mathbb{R} are distributions of self-adjoint operators and a sum of self-adjoint operators is again such an operator, the additive free convolution \boxplus yields an operation on probability measures on \mathbb{R} . Similarly, it can be shown that \boxtimes gives rise to operations on probability measures on $\{z \in \mathbb{C} \mid |z|=1\}$ and on probability measures on $[0, \infty)$.

With the R -transform machinery at hand, the free analogs of many of the classical results around addition of independent random variables have been developed (we recommend Voiculescu (1998c) for a survey of these developments). This includes the classification of infinitely divisible laws (Levy–Khintchine type theorem), classification of stable laws, domains of attraction, and convolution semigroups. Note that the free laws are rather different from the classical ones, but the classification results are quite parallel, that is, the indexing parameters are almost the same. The situation is similar in the multiplicative context. As in the classical case, these results about laws yield in particular processes with independent increments, which in the free framework are free increments.

As in the classical setting, also in the free setting, convolution semigroups are connected to differential

equations. In the additive free case, a semigroup is a family $(\mu_t)_{t \geq 0}$ of probability measures on \mathbb{R} , so that $\mu_{t+s} = \mu_t \boxplus \mu_s$. If $G(t, z)$ is the Cauchy transform of μ_t (which is an analytic function on the half-plane $\text{Im } z > 0$), the equation (Voiculescu 1986) is a semilinear complex PDE:

$$\frac{\partial G}{\partial t} + R_{\mu_1}(G) \frac{\partial G}{\partial z} = 0$$

where R_{μ_1} is the R -transform of μ_1 . In particular, when μ_1 is the semicircle law, $R_{\mu_1}(z) = \alpha z$ $\alpha > 0$ and the PDE is a complex Burgers equation in the upper half-plane.

Noncrossing Partitions

The series expansion of the R -transform

$$R_\mu(z) = \sum_{n \geq 0} R_n(\mu) z^n$$

has as coefficients polynomials $R_n(\mu)$ in the moments $\mu(X^k)$. More precisely, assigning to $\mu(X^k)$ a degree k , $R_n(\mu)$ is a polynomial of degree n and $R_n(\mu) - \mu(X^n)$ is polynomial in $\mu(X^k)$ with $k < n$. The linearization property of the R -transform implies that

$$R_n(\mu \boxplus \nu) = R_n(\mu) + R_n(\nu)$$

For classical convolution, polynomials with similar properties satisfying

$$C_n(\mu * \nu) = C_n(\mu) + C_n(\nu)$$

are called cummulants and satisfy

$$\log \mu(e^{zX}) = \sum_{n \geq 1} C_n(\mu) z^n$$

There are combinatorial formulas involving the lattice of all partitions of the set $\{1, \dots, n\}$ which give the classical cummulants. For free cummulants, like $R_n(\mu)$ and generalizations of these, there are similar formulas provided the lattice of all partitions is replaced by the lattice $\text{NC}(n)$ of noncrossing partitions (Speicher 1998). A partition $\pi = (V_1, \dots, V_m)$ of $\{1, \dots, n\}$ is noncrossing if there are no $a < b < c < d$ so that $\{a, c\} \subset V_k$, $\{b, d\} \subset V_l$ and $k \neq l$.

More generally, a family $R^{(n)}(a_1, \dots, a_n)$ of free cummulants, where a_1, \dots, a_n are in some (A, φ) , is defined recursively as follows (Speicher 1998). For $n=1$, one has $R^{(1)}(a) = \varphi(a)$. If $\pi = (V_1, \dots, V_m) \in \text{NC}(n)$, where $V_k = \{i(1, k) < \dots < i(n_k, k)\}$, we define

$$R[\pi](a_1, \dots, a_n) = \prod_{1 \leq k \leq m} R^{(|V_k|)}(a_{i(1,k)}, \dots, a_{i(n_k,k)})$$

The recurrence relation for cumulants is then

$$\varphi(a_1 \dots a_n) = \sum_{\pi \in \text{NC}(n)} R[\pi](a_1, \dots, a_n)$$

Note that the right-hand side involves only $R^{(k)}$'s with $k \leq n$ and that actually $R^{(n)}$ appears only in and is equal to $R[\{1, \dots, n\}](a_1, \dots, a_n)$ (the coarsest partition).

A key property of $R^{(n)}(a_1, \dots, a_n)$ is that if $\{1, \dots, n\} = \alpha \amalg \beta$ and $(a_k)_{k \in \alpha}, (a_l)_{l \in \beta}$ are freely independent, then $R^{(n)}(a_1, \dots, a_n) = 0$.

If μ is the distribution of $a \in (A, \varphi)$, then the cumulants $R_n(\mu)$ are given by

$$R_n(\mu) = R^{(n)}(a, \dots, a)$$

The noncrossing condition on partitions corresponds to a planarity requirement for diagrams and as such is very suggestive of connections to planar diagrams occurring in the constant term of large- N expansions from random matrix theory and more generally gauge theory.

For more details on the subject of noncrossing partitions, we refer the reader to the memoir by Speicher (1998).

Asymptotic Freeness of Random Matrices

The explanation for the coincidences between certain laws in free probability and in random matrix theory is that freeness occurs asymptotically among random matrices in the large- N limit (Voiculescu 1991).

Random matrices can be put in a noncommutative probability framework $(\mathcal{A}_N, \varphi_N)$, where $\mathcal{A}_N = L^{\infty-0}(\Omega, \mathcal{M}_N; d\sigma)$ (the $N \times N$ complex matrix-valued functions on the probability space $(\Omega, d\sigma)$ which are p -integrable for all $p \in [1, \infty)$) and the expectation functional is

$$\varphi_N(X) = N^{-1} \int_{\Omega} \text{tr } X(\omega) d\sigma(\omega)$$

The basic example is provided by an n -tuple of Gaussian random matrices (Voiculescu 1991). Let

$$T_j^{(N)} = (a_{p,q;j}^{(N)})_{1 \leq p,q \leq N} \in \mathcal{M}_N, \quad 1 \leq j \leq n$$

where $a_{p,q;j}^{(N)} = a_{q,p;j}^{(N)}$ and the $a_{p,q;j}^{(N)}, 1 \leq p \leq q \leq N, 1 \leq j \leq n$ are $(0, N^{-1})$ -Gaussian and independent. Then $(T_j^{(N)})_{1 \leq j \leq n}$ as $N \rightarrow \infty$ converges in noncommutative distribution to the freely independent n -tuple $(l(e_j) + l^*(e_j))_{1 \leq j \leq n}$ in the Boltzmann Fock space

context of Example 2 for an orthonormal system $e_1, \dots, e_n \in \mathcal{H}$, that is, convergence of moments:

$$\begin{aligned} \lim_{N \rightarrow \infty} \varphi_N(T_{i_1}^{(N)} \dots T_{i_k}^{(N)}) \\ = \langle (l(e_{i_1}) + l^*(e_{i_1})) \dots (l(e_{i_k}) + l^*(e_{i_k})) 1, 1 \rangle \end{aligned}$$

In particular, the limit variables $(l(e_j) + l^*(e_j))_{1 \leq j \leq n}$ are free.

More generally, asymptotic freeness of variables or sets of variables in $(\mathcal{A}_N, \varphi_N)$ can be defined without the existence of a limit distribution, that is, by requiring only that the freeness relations among noncommutative moments hold asymptotically as $N \rightarrow \infty$.

Note that in these random matrix questions, the joint classical distribution of an n -tuple of random matrices $(X_1^{(N)}, \dots, X_n^{(N)})$ in \mathcal{A}_N is a probability measure on $(\mathcal{M}_N)^n$ which contains more information than the collection of noncommutative moments, which is the distribution of the noncommutative variables in $(\mathcal{A}_N, \varphi_N)$. In particular, for one random matrix the classical distribution gives the joint distribution of all entries, whereas the noncommutative distribution gives information only about the distribution of eigenvalues.

From the Gaussian n -tuple using operator techniques much more general asymptotic freeness results have been obtained. For instance (Voiculescu 1998b):

Let $(X_1^{(N)}, \dots, X_m^{(N)}, Y_1^{(N)}, \dots, Y_n^{(N)})$ be $(m+n)$ -tuples of self-adjoint $N \times N$ random matrices with classical joint distribution μ_N on $(\mathcal{M}_N^{\text{sa}})^{m+n}$. Assume that μ_N is invariant under the action of the unitary group $U(N)$ which takes $(X_1, \dots, X_m, Y_1, \dots, Y_n)$ into $(X_1, \dots, X_m, UY_1U^*, \dots, UY_nU^*)$ and assume that there is a bound R on the operator norms $\|X_j^{(N)}\|$ and $\|Y_j^{(N)}\|$ independent of N . Then the sets $\{X_1^{(N)}, \dots, X_m^{(N)}\}$ and $\{Y_1^{(N)}, \dots, Y_n^{(N)}\}$ are asymptotically free as $N \rightarrow \infty$.

Note that the uniform bound on the operator norms can be easily replaced by weaker conditions.

Once we know that certain random matrices are asymptotically free and that the large- N limit in noncommutative distribution exists, the results of free probability apply. For instance, if $X^{(N)}$ and $Y^{(N)}$ are asymptotically free and have limit distributions μ and ν , then the limit distribution of $X^{(N)} + Y^{(N)}$ and of $X^{(N)} Y^{(N)}$ are the free convolutions $\mu \boxplus \nu$ and, respectively, $\mu \boxtimes \nu$.

Free probability techniques have also been successful in dealing with other questions about the asymptotic behavior of random matrices.

If $T_1^{(N)}, \dots, T_n^{(N)}$ is an n -tuple of i.i.d. Hermitian Gaussian random, then the uniform operator norms

of polynomials in noncommutative indeterminates have the property that

$$\lim_{N \rightarrow \infty} \|P(T_1^{(N)}, \dots, T_n^{(N)})\| \\ = \|P(l(e_1) + l(e_1)^*, \dots, l(e_n) + l(e_n)^*)\|$$

almost surely (Haagerup and Thorbjørnsen).

This result is a far-reaching generalization of the results about largest eigenvalues of one Gaussian random matrix. The use of operator-valued free random variables (with respect to certain subalgebra) was an essential ingredient in the proof. Also, in another direction, freeness of operator-valued free random variables was used to obtain a free probability treatment of Gaussian random band matrices and generalizations of these (Shlyakhtenko 1996).

Finally, quite recently, extensions of the free probability framework have appeared which are adapted to the study of fluctuations of systems of random matrices in the large- N limit.

Free Entropy

There are free probability analogs also for information-theoretic quantities (Voiculescu 1994, 1998a).

Let (f_1, \dots, f_n) be an n -tuple of classical numerical random variables the joint distribution of which has density $p(t_1, \dots, t_n)$ with respect to the n -dimensional Lebesgue measure λ_n on \mathbb{R}^n . The entropy quantity associated by Shannon to (f_1, \dots, f_n) is

$$H(f_1, \dots, f_n) = - \int_{\mathbb{R}^n} p \log p \, d\lambda_n$$

The free analog of $H(f_1, \dots, f_n)$ is the free entropy quantity $\chi(X_1, \dots, X_n)$. Here $X_j = X_j^*$, $1 \leq j \leq n$, are noncommutative self-adjoint random variables in (M, τ) , where M is a $*$ -algebra of bounded operators on a Hilbert space \mathcal{H} . The expectation functional in addition to the positivity properties, equivalent to the requirement that it can be defined by a unit vector $\tau(\cdot) = \langle \cdot, \xi \rangle$, also has the property of a trace $\tau(XY) = \tau(YX)$ for all $X, Y \in M$. For instance, the noncommutative random variables arising from the large- N limit of n -tuples of self-adjoint random matrices live in noncommutative probability frameworks (M, τ) of this kind.

There are two approaches to defining free entropy and, since there are only partial results about the equivalence of these approaches, the quantities obtained are denoted by $\chi(X_1, \dots, X_n)$ (Voiculescu 1994) and $\chi^*(X_1, \dots, X_n)$ (Voiculescu 1998a). The quantity χ is often referred to as the “microstates free entropy,” its definition being inspired by the Boltzmann formula $S = k \log W$, whereas the other entropy, sometimes called “microstates-free free

entropy,” is obtained via a free probability analog of the Fisher information (Voiculescu 1998a).

The microstates used to define χ are matricial and the reason why this choice produced a quantity with the right behavior with respect to free independence can be found in the asymptotic freeness properties of random matrices.

Given $X_j = X_j^* \in M$, $1 \leq j \leq n$ and $m \in \mathbb{N}$, $k \in \mathbb{N}$, $\epsilon > 0$ the microstates $\Gamma(X_1, \dots, X_n; m, k, \epsilon)$ are n -tuples (A_1, \dots, A_n) of self-adjoint $k \times k$ matrices, such that, for noncommutative moments of order up to m , we have

$$|k^{-1} \text{tr}_k(A_{i_1} \dots A_{i_p}) - \tau(X_{i_1} \dots X_{i_p})| < \epsilon$$

where $1 \leq p \leq m$, $1 \leq i_j \leq n$, $1 \leq j \leq p$.

One obtains $\chi(X_1, \dots, X_n)$ by taking the infimum over $\epsilon > 0$ and $m \in \mathbb{N}$ of

$$\limsup_{k \rightarrow \infty} \left(k^{-2} \log \text{vol } \Gamma(\dots) + \frac{n}{2} \log k \right)$$

where vol is the volume on $(\mathcal{M}_k^{\text{sa}})^n$ corresponding to the Hilbert–Schmidt norm Hilbert space structure (Voiculescu 1994).

When $n = 1$, there is a simple formula for $\chi(X)$. If μ is the probability measure on \mathbb{R} which represents the distribution of $X = X^* \in M$ with respect to the expectation τ , then

$$\chi(X) = \iint \log |s - t| d\mu(s) d\mu(t) + C$$

where the exact value of the constant C is $3/4 + 1/2 \log 2\pi$.

For $n > 1$ there is no simple formula for $\chi(X_1, \dots, X_n)$, but there are several properties which provide a better understanding of this quantity.

If X_j are such that $\chi(X_j) > -\infty$, then

$$\chi(X_1, \dots, X_n) = \chi(X_1) + \dots + \chi(X_n)$$

if and only if X_1, \dots, X_n are freely independent in (M, τ) . Clearly, this property of χ with respect to free independence is analogous to the property of $H(f_1, \dots, f_n)$ with respect to classical independence.

Further, if F_1, \dots, F_n are power series in n noncommuting indeterminates, there is a change-of-variable formula

$$\chi(F_1(X_1, \dots, X_n), \dots, F_n(X_1, \dots, X_n)) \\ = \log |\det(\mathcal{J}(F))| + \chi(X_1, \dots, X_n)$$

involving the Kadison–Fuglede positive determinant $|\det|$ and a certain noncommutative Jacobian $\mathcal{J}(F)$, $F = (F_1, \dots, F_n)$ defined in $\mathcal{M}_n \otimes M \otimes M^{\text{op}}$, where M^{op} is the opposite algebra of M . (For

definitions and the many technical conditions under which this formula holds, see Voiculescu (1994).)

The free entropy χ also satisfies semicontinuity, subadditivity, and a semicircular bound (analogous to the classical Gaussian bound) properties.

An unexpected feature of χ is a degeneration of convexity. If the trace state τ is a convex combination $\tau = \theta\tau' + (1 - \theta)\tau''$, where τ', τ'' are trace states and where $\tau' \neq \tau''$ on the algebra generated by X_1, \dots, X_n , and $n > 1$, then

$$\chi(X_1, \dots, X_n) = -\infty$$

(for a reference consult the survey Voiculescu (2002)).

With the free entropy at hand, an important variational problem can be formulated for the noncommutative distribution of an n -tuple of self-adjoint noncommutative random variables T_1, \dots, T_n in the tracial context. The quantity to be maximized is

$$\chi(T_1, \dots, T_n) - \tau(P(T_1, \dots, T_n))$$

where P is a given self-adjoint polynomial in noncommutative indeterminates (see Voiculescu (2002) for comments on this problem). If $n = 1$, this is a classical problem for the logarithmic energy

$$\iint \log |s - t| d\mu(s) d\mu(t) - \int P(t) d\mu(t)$$

where μ is a probability measure on \mathbb{R} .

To explain the second approach, based on Fisher information, we begin by recalling some facts about Fisher information in the classical context.

If f is a numerical random variable with distribution given by the density $p(t)$ on \mathbb{R} , then

$$\text{Fisher}(f) = \int \left(\frac{-p'}{p} \right)^2 p dt = \left\| \left(\frac{d}{dt} \right)^* 1 \right\|_{L^2(\mathbb{R}, p dt)}$$

Here d/dt is the differential operator defined on test functions in $L^2(\mathbb{R}, p dt)$. Then

$$\frac{p'}{p} = - \left(\frac{d}{dt} \right)^* 1$$

The classical connection to entropy is that the Fisher information is a derivative of the entropy when the variable becomes the starting point of a Brownian motion. This can be written as

$$\text{Fisher}(f) = \frac{d}{dt} H(f + t^{1/2}g) \Big|_{t=0}$$

where g and f are independent and g is $(0, 1)$ Gaussian.

The several-variables version is treated by using partial derivatives.

The analog in free probability of the Fisher information (Voiculescu 1998a) is obtained by using the free difference quotient derivations, which are the appropriate derivations in this maximally noncommutative setting. On the polynomials in n noncommutative indeterminates, the k th partial free difference quotient

$$\partial_k : C\langle X_1, \dots, X_n \rangle \rightarrow C\langle X_1, \dots, X_n \rangle^{\otimes 2}$$

is defined on noncommutative monomials by the formula

$$\partial_k X_{i_1} \cdots X_{i_p} = \sum_{\{j|i_j=k\}} X_{i_1} \cdots X_{i_{j-1}} \otimes X_{i_{j+1}} \cdots X_{i_p}$$

If $X_j = X_j^*$, $1 \leq j \leq n$, are noncommutative random variables in (M, τ) , which do not satisfy any nontrivial algebraic relations, to simplify matters we can assume that M is generated by X_1, \dots, X_n and identify M with $C\langle X_1, \dots, X_n \rangle$. The trace state τ gives rise to a scalar product $\langle m_1, m_2 \rangle = \tau(m_2^* m_1)$ on M . Let $L^2(M, \tau)$ denote the Hilbert space obtained from M . Then, skipping some technicalities, ∂_k will give rise to a densely defined operator of $L^2(M, \tau)$ into $L^2(M, \tau) \otimes L^2(M, \tau)$. If $1 \otimes 1$ is in the domain of the adjoints ∂_k^* , the free Fisher information of the n -tuple X_1, \dots, X_n is defined to be

$$\Phi^*(X_1, \dots, X_n) = \sum_{1 \leq k \leq n} \|\partial_k^*(1 \otimes 1)\|_{L^2(M, \tau)}^2$$

In case $1 \otimes 1$ is not in the domain of some ∂_k^* , the free Fisher information is given the value ∞ .

The “microstates-free free entropy” χ^* is then defined by

$$\begin{aligned} \chi^*(X_1, \dots, X_n) = & \frac{n}{2} \log 2\pi e \\ & + \int_0^\infty \left(\frac{n}{1+t} - \Phi^* \right. \\ & \left. \times (X_1 + t^{1/2}S_1, \dots, X_n + t^{1/2}S_n) \right) dt \end{aligned}$$

where S_1, \dots, S_n are $(0, 1)$ -semicircular and freely independent and also freely independent of $\{X_1, \dots, X_n\}$.

For $n = 1$ it is known that $\chi^*(X) = \chi(X)$ and the free Fisher information is

$$\Phi^*(X) = \frac{2\pi^2}{3} \int p^3(t) dt$$

if $p(t)$ is the density with respect to the Lebesgue measure of the distribution of X . The computation of $\partial^* 1 \otimes 1$ is possible in the one-variable case and up to a factor the result is $(Hp)(X)$, where Hp is the Hilbert transform of p .

Several of the classical inequalities for the Fisher information have free probability analogs (Voiculescu 1998a) (Cramer–Rao inequality, Stam inequality, information-log-Sobolev inequality, and others).

For $n > 1$ only $\chi \leq \chi^*$, the easier of the inequalities among χ and χ^* , has been established (Biane *et al.* 2003). This result was obtained based on an important connection of χ and χ^* to large deviations. The deviations studied are for the noncommutative distributions of n -tuples of matrices in the case of an n -tuple of Gaussian random matrices. In this context χ is related to the quantity to be estimated and χ^* is related to the rate function.

For more details on free entropy, the reader is referred to the survey articles by Voiculescu (1998c, 2002).

Concluding Comments

For more details, additional results, and bibliography, we refer the reader to the expositions in Voiculescu (1998c), Voiculescu *et al.* (1992) and Speicher (1998). To get even more detail, the reader may consult, besides the original papers of the present author, those of P Biane, R Speicher, D Shlyakhtenko, K J Dykema, A Nica, U Haagerup, H Bercovici, L Ge, F Radulescu, A Guionnet, T Cabanal–Duvillard, M Anshelevich, to name a few of the main contributors.

Also, via random matrices, there are connections to physics models (especially large- N 2D Yang–Mills QCD) in work of I M Singer, M Douglas, D Gross–R Gopakumar, P Zinn–Justin. In a loose sense, one may view the noncrossing partitions combinatorics as related to the work on planar diagrams and the large- N limit of t’Hooft and Brezin–Itzykson–Parisi–Zuber in the 1970s.

See also: Large Deviations in Equilibrium Statistical Mechanics; Large- N and Topological Strings; Random Matrix Theory in Physics.

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Functional Equations and Integrable Systems

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Introduction

Functional equations have a long and interesting history in connection with mathematical physics and touch upon many branches of mathematics. They have arisen in the context of both classical and quantum completely integrable systems in several different ways and we shall survey some of these.

In the great majority of cases functional equations appear in the integrable system setting as the result of an ansatz: a particular form of a solution is either guessed or postulated, the consistency of which yields a functional equation. What the ansatz is for can vary significantly. As outlined below, amongst others, one may postulate algebraic structures in the form of the existence of a Lax pair or of conserved quantities; in the quantum setting, one may postulate properties of a ground-state wave function or the ring of commuting differential operators. Appearing in this way, functional equations are really just another of the (significant) tools-of-the-trade for constructing and discovering new integrable systems. However, as one surveys both the functional equations and the functions they describe one sees certain common features. The functions are most frequently associated with an elliptic curve, a genus-1 abelian variety. One can seek to associate these to another fundamental ingredient of modern integrable systems, the Baker–Akhiezer function. Indeed, very few of the ansätze made directly suggest that the systems being constructed will be completely integrable. This very desirable property usually is a bonus of the construction and hints of more fundamental connections. Another fundamental connection we shall mention is that with topology. The phase space of a completely integrable system is rather special, admitting (generically) a foliation by tori. The functional equations we encounter often also characterize the Hirzebruch genera associated with the index theorems of known elliptic operators. These are typically evaluated by Atiyah–Bott fixed-point theorems for circle actions on the manifold. A general understanding of the various interconnections has yet to be achieved.

To bring to focus our discussion we shall concentrate on functional equations arising from studying systems with an arbitrary number of particles (n below). In principle, there could be many different interactions between the particles and symmetry will

be used to limit these. The use of symmetry is a key ingredient, often implicit, in the various ansätze we shall describe. For simplicity, we shall most often focus on the situation where the particles are identical. In algebraic terms, we focus on the symmetric group S_n and root systems of type a_n ; generalizations frequently exist for other root systems and Weyl groups and we shall simply note this at the outset.

Lax Pairs

The modern approach to integrable systems is to utilize a Lax pair, that is, a pair of matrices L, M such that the zero curvature condition $\dot{L} = [L, M]$ is equivalent to the equations of motion. By construction, Lax pairs produce the conserved quantities $\text{tr } L^k$. To establish integrability, one must further show both that there are enough functionally independent conserved quantities and that these are in involution. (R -matrices are the additional ingredient of the modern approach to establishing involutivity.) Lax pairs can fail on both counts, and so the construction of a Lax pair is but the first step in establishing a system to be completely integrable. The great merit of the modern approach is that it provides a unified framework for treating the many disparate completely integrable systems known. Unfortunately the construction of a Lax pair is often far from straightforward and typically hides the “clever tricks” frequently employed in establishing integrability. In the present context, we shall outline how functional equations have been used to construct Lax pairs. The paradigm for this approach is the Calogero–Moser system.

Beginning with the ansatz (for $n \times n$ matrices)

$$L_{jk} = p_j \delta_{jk} + g(1 - \delta_{jk})A(q_j - q_k)$$

$$M_{jk} = g \left[\delta_{jk} \sum_{l \neq j} B(q_j - q_l) - (1 - \delta_{jk})C(q_j - q_k) \right]$$

one finds $\dot{L} = [L, M]$ yields the equations of motion for the Hamiltonian system ($n \geq 3$)

$$H = \frac{1}{2} \sum_j p_j^2 + g^2 \sum_{j < k} U(q_j - q_k) \quad [1]$$

$$U(x) = A(x)A(-x) + \text{const.}$$

provided $C(x) = -A'(x)$, and that $A(x)$ and $B(x)$ satisfy the functional equation

$$A(x+y)[B(x) - B(y)] = A(x)A'(y) - A(y)A'(x) \quad [2]$$

This is a particular example of a more general functional equation whose solution will be described

below. For the present, we simply note that for this system the corresponding potential is the Weierstrass \wp -function, $A(x)A(-x) = \wp(\nu) - \wp(x)$, and the resulting Hamiltonian system [1] is known as the Calogero–Moser system. It is completely integrable though, as already remarked, the ansatz did not necessitate this. The Lax pair presented here and the reduction of its consistency to a functional equation and algebraic constraints follows Calogero (1976) in which he discovered the elliptic generalization of the model he had introduced in 1975.

A different ansatz for a Lax pair is

$$L_{jk} = \dot{q}_j \delta_{jk} + (1 - \delta_{jk}) \sqrt{\dot{q}_j \dot{q}_k} A(q_j - q_k)$$

$$M_{jk} = \delta_{jk} \sum_{l \neq j} \dot{q}_l B(q_j - q_l) + (1 - \delta_{jk}) \sqrt{\dot{q}_j \dot{q}_k} C(q_j - q_k)$$

Now the consistency of the Lax pair yields equations of motion of the form

$$\ddot{q}_j = \sum_{k \neq j} \dot{q}_j \dot{q}_k V(q_j - q_k)$$

$$V(x) = \begin{vmatrix} A(x) & A(-x) \\ C(x) & C(-x) \end{vmatrix} = -V(-x)$$

provided $B(x) = B(-x)$, $C(x) = A'(x) - A(x)G(x)$, where we have defined $G(x) = B(x) + (1/2)V(x)$, and the functions satisfy the functional equation

$$A(x+y) = A(x)A(y) + \frac{\begin{vmatrix} A(x) & A(y) \\ A'(x) & A'(y) \end{vmatrix}}{G(x) - G(y)}$$

$$= \frac{\begin{vmatrix} A(x) & A(y) \\ C(x) & C(y) \end{vmatrix}}{G(x) - G(y)} \quad [3]$$

Again we shall briefly defer describing the solution of this equation and simply note that the general solution for $V(x)$ is again given in terms of the Weierstrass \wp -function $V(x) = \wp'(x)/(\wp(\nu) - \wp(x))$ and that the equations of motion follow from the Hamiltonian

$$H = \sum_j e^{p_j} \prod_{k \neq j} \sqrt{\wp(\nu) - \wp(q_j - q_k)}$$

This is known as the Ruijsenaars–Schneider model and it too is completely integrable. The Lax pair here was constructed by Bruschi and Calogero.

In the two examples of Lax pairs just presented, each particle interacts with every other pairwise. By modifying the ansatz, it is possible to construct models that interact with just their nearest neighbors (which include the Toda systems). More generally,

an ansatz exists for a Lax pair associated with equations of motion of the form

$$\ddot{q}_j = \sum_{k \neq j} (a + b\dot{q}_j)(a + b\dot{q}_k) V_{jk}(q_j - q_k) \quad [4]$$

which unifies, for example, the Calogero–Moser, Ruijsenaars–Schneider, and Toda systems. The functional equations now encountered are typically (and whenever $b \neq 0$) of the form

$$\phi_1(x+y) = \frac{\begin{vmatrix} \phi_2(x) & \phi_2(y) \\ \phi_3(x) & \phi_3(y) \\ \phi_4(x) & \phi_4(y) \\ \phi_5(x) & \phi_5(y) \end{vmatrix}}{\begin{vmatrix} \phi_4(x) & \phi_4(y) \\ \phi_5(x) & \phi_5(y) \end{vmatrix}} \quad [5]$$

This functional equation, for five *a priori* unknown functions, includes [2] and [3] as special cases.

The general analytic solution of [5] is, up to symmetries, given by

$$\phi_1(x) = \frac{\Phi(x; \nu_1)}{\Phi(x; \nu_2)}, \quad \begin{pmatrix} \phi_2(x) \\ \phi_3(x) \end{pmatrix} = \begin{pmatrix} \Phi(x; \nu_1) \\ \Phi'(x; \nu_1) \end{pmatrix}$$

$$\begin{pmatrix} \phi_4(x) \\ \phi_5(x) \end{pmatrix} = \begin{pmatrix} \Phi(x; \nu_2) \\ \Phi'(x; \nu_2) \end{pmatrix}$$

where

$$\Phi(x; \nu) \equiv \frac{\sigma(\nu - x)}{\sigma(\nu)\sigma(x)} e^{\zeta(\nu)x} \quad [6]$$

Here, $\zeta(x) = \sigma(x)'/\sigma(x)$ is the Weierstrass ζ -function. The solution of [2] arises as the $\nu_2 \rightarrow 0$ limit of [5].

The proof of the general solution just stated is in fact constructive (Braden and Buchstaber 1997). The parameters appearing in the solution are determined as follows. Suppose x_0 is a generic point for [5]. Then (for $k=1, 2$), we have that

$$\partial_y \ln \left| \begin{vmatrix} \phi_{2k}(x+x_0) & \phi_{2k}(y+x_0) \\ \phi_{2k+1}(x+x_0) & \phi_{2k+1}(y+x_0) \end{vmatrix} \right|_{y=0}$$

$$= \zeta(\nu_k) - \zeta(x) - \zeta(\nu_k - x) - \lambda_k$$

$$= -\frac{1}{x} - \lambda_k + \sum_{l=0} F_l \frac{x^{l+1}}{(l+1)!} \quad [7]$$

The Laurent expansion determines the parameters g_1, g_2 (which are the same for both $k=1, 2$) characterizing the elliptic functions of [6] by

$$g_2 = \frac{5}{3}(F_2 + 6F_0^2), \quad g_3 = 6F_0^3 - F_1^2 + \frac{5}{3}F_0F_2$$

and the parameters ν_k via $F_0 = -\wp(\nu_k)$. Here, $\wp(x) = -\zeta'(x)$ is the Weierstrass elliptic \wp -function

with periods $2\omega, 2\omega'$ that satisfies the differential equation

$$\wp'(x)^2 = 4\wp(x)^3 - g_2\wp(x) - g_3$$

The constructive nature of the solutions of [5] means that it is straightforward to construct solutions to various specializations of the equation such as

$$\phi_1(x+y) = \phi_4(x)\phi_5(y) + \phi_4(y)\phi_5(x)$$

(obtained by requiring $\phi_2(x) = \phi_4^2(x)$ and $\phi_3(x) = \phi_5^2(x)$). More complicated functional equations such as

$$\begin{aligned} \Psi_1(x+y) = & \Psi_2(x+y)\phi_2(x)\phi_3(y) \\ & + \Psi_3(x+y)\phi_4(x)\phi_5(y) \end{aligned} \quad [8]$$

may be solved using the solutions of [5].

Finally, let us note that the general system [4] may lead to functional equations not just of the form [5], for example,

$$\begin{aligned} \phi_6(x+y) = & \phi_1(x+y)(\phi_4(x) - \phi_5(y)) \\ & + \begin{vmatrix} \phi_2(x) & \phi_3(y) \\ \phi_2'(x) & \phi_3'(y) \end{vmatrix} \end{aligned} \quad [9]$$

The general analytic solution to [9] has yet to be determined although particular solutions are known.

As a final example of a functional equation coming from an ansatz for a Lax pair, consider

$$L_{jk} = \sqrt{p_j p_k} A(q_j - q_k), \quad M_{jk} = \sqrt{p_j p_k} C(q_j - q_k)$$

where we now assume $A(0)$ and $C(0)$ regular. Then the consistency of this Lax pair corresponds to the equations of motion for the Hamiltonian

$$H = \sum_{j,k} p_j p_k f(q_j - q_k) \quad [10]$$

provided f is even and the functional equation

$$\begin{aligned} 2A'(x+y)[f(x) - f(y)] \\ - A(x+y)[f'(x) - f'(y)] = \begin{vmatrix} A(x) & A(y) \\ C(x) & C(y) \end{vmatrix} \end{aligned} \quad [11]$$

is satisfied. The Hamiltonian system [10] corresponds to geodesic motion. Nonanalytic solutions are known to the functional equation [11].

An Algebraic Ansatz: Conserved Quantities

Another way in which functional equations may appear is by making an ansatz for an additional conserved quantity beyond the Hamiltonian. For two

and three particles on the line, Hietarinta derived functional equations by seeking a second quartic or cubic integral (respectively). Here, a key ingredient is the assumption of a further invariant polynomial in the momenta. Polynomial invariance, together with symmetry, is quite constraining. Consider

Theorem 1 *Let H and P be the (natural) Hamiltonian and center of mass momentum*

$$H = \frac{1}{2} \sum_{i=1}^n p_i^2 + V, \quad P = \sum_{i=1}^n p_i$$

Denote by Q an independent third-order quantity

$$\begin{aligned} Q = & \sum_{i=1}^n p_i^3 + \frac{1}{6} \sum_{i \neq j \neq k} d_{ijk} p_i p_j p_k + \sum_{i \neq j} d_{ij} p_i^2 p_j \\ & + \frac{1}{2} \sum_{ij} a_{ij} p_i p_j + \sum_i b_i p_i + c \end{aligned}$$

If these are S_n -invariant and Poisson-commute,

$$\{P, H\} = \{P, Q\} = \{Q, H\} = 0$$

then

$$V = \frac{1}{6} \sum_{i \neq j} \wp(q_i - q_j) + \text{const.}$$

and we have the Calogero–Moser system.

Here, the symmetric group invariance means that for any coefficient $\alpha_{ij}(q_1, q_2, \dots, q_n)$ in the expansions above, we have $\alpha_{\sigma(i)\sigma(j)}(q_{\sigma(1)}, q_{\sigma(2)}, \dots, q_{\sigma(n)})$ for all $\sigma \in S_n$. In particular, $V(q_1, q_2, \dots, q_n) = V(q_{\sigma(1)}, q_{\sigma(2)}, \dots, q_{\sigma(n)})$ for all $\sigma \in S_n$. We remark that had we begun with particles of possibly different particle masses, $H = (1/2) \sum_{i=1}^n m_i p_i^2 + V$; the effect of S_n -invariance is such as to require these masses to be the same. Thus, we are assuming the S_n -invariant Hamiltonian of the theorem. Finally, by “an independent third-order quantity” Q , we mean one functionally independent of H and P and for which one cannot obtain an invariant of lower degree by subtracting multiples of P^3 and PH . We are not dealing with quadratic conserved quantities here.

The assumed polynomial behavior of the conserved quantities means that when calculating Poisson brackets, the coefficients of independent monomials must vanish. This, together with symmetry, leads to the functional equation

$$\begin{vmatrix} 1 & 1 & 1 \\ F(x) & F(y) & F(z) \\ F'(x) & F'(y) & F'(z) \end{vmatrix} = 0, \quad x + y + z = 0 \quad [12]$$

The result follows in light of

Theorem 2 *Let f be a three-times differentiable function satisfying the functional equation [12]. Up to the manifest invariance*

$$F(x) \rightarrow \alpha F(\delta x) + \beta$$

the solutions of [12] are one of $F(x) = \wp(x + d)$, $F(x) = e^x$ or $F(x) = x$. Here, \wp is the Weierstrass \wp -function and $3d$ is a lattice point of the \wp -function.

Again we note that the ansatz *per se* has not established complete integrability: the ansatz leads us to the Calogero–Moser model whose complete integrability must be established by other means. This result may be interpreted as a rigidity theorem for the a_n Calogero–Moser system and in part explains this models' ubiquity: demanding a cubic invariant together with S_n -invariance necessitates the model. A natural generalization is to replace the S_n -invariance with the invariance of a general Weyl group W and make connection with the Calogero–Moser models associated to other root systems (Perelomov 1990).

We shall encounter the functional equation [12] again in this survey and now note that this may be generalized to

$$\begin{vmatrix} 1 & 1 & 1 \\ F(x) & G(y) & H(z) \\ F'(x) & G'(y) & H'(z) \end{vmatrix} = 0, \quad x + y + z = 0 \quad [13]$$

If F, G , and H are three-times differentiable functions satisfying the functional equation [13], then, up to the manifest invariance,

$$F(x) \rightarrow \alpha F(\delta x + \gamma_1) + \beta$$

$$G(x) \rightarrow \alpha G(\delta x + \gamma_2) + \beta$$

$$H(x) \rightarrow \alpha H(\delta x + \gamma_3) + \beta$$

where $\gamma_1 + \gamma_2 + \gamma_3 = 0$, the nonconstant solutions of [13] are given by $F(x) = G(x) = H(x) = e^x$, x , or $\wp(x)$. If (say) $H(z)$ is a constant then either

1. one of the functions $F(x)$ or $G(y)$ is the same constant as $H(z)$, in which case the remaining function is arbitrary, or
2. $F(x) = G(x) = e^x$.

We remark that in fact the exponential and linear function solutions satisfy [12] and [13] without the constraint $x + y + z = 0$. Further, the theorems immediately give the general analytic solutions to

the same functional equations viewed as functions of a complex variable, showing that the solutions are in fact meromorphic. These theorems were established in Braden and Byatt-Smith (1999) where earlier results are described.

Quantum Calogero–Moser Systems

Quite a bit is known about the quantum generalizations of the Calogero–Moser system. The polynomial and Weyl group W -invariance of the classical conserved quantities is replaced by a commutative ring \mathcal{R} of W -invariant, holomorphic, differential operators, whose highest-order terms generate W -invariant differential operators with constant coefficients. The Poisson bracket is then replaced by a commutator of operators. When this is done functional equations again ensue and one finds that the potential term for the Laplacian \mathcal{H} (the quantum Hamiltonian) has Calogero–Moser potential appropriate to W (Oshima and Sekiguchi 1995). In this setting, it is known that the commutativity of just a few low-order elements of \mathcal{R} dictate the form of the potential and the commuting algebra (at least for the classical root systems). In particular, Theorem 1 above is the classical analog for the a_n root system of a quantum result where a functional equation equivalent to [12] was obtained by requiring the commutativity of certain linear, quadratic, and cubic holomorphic differential operators. Taniguchi's results (Taniguchi 1997) are also indicative of the rigidity of these quantum models: if \mathcal{H} is the quantum Hamiltonian just discussed, and $\mathcal{Q}_{1,2}$ are holomorphic (but not *a priori* W -invariant), differential operators of appropriate degrees for which $[\mathcal{Q}_{1,2}, \mathcal{H}] = 0$, then $\mathcal{Q}_{1,2} \in \mathcal{R}$ and consequently $[\mathcal{Q}_1, \mathcal{Q}_2] = 0$.

An Algebraic Ansatz: The Poincaré Algebra

We have earlier encountered the Ruijsenaars–Schneider models when considering functional equations ensuing from ansatz for Lax pairs. These models were however discovered by another route (Ruijsenaars and Schneider 1986) in the course of investigating mechanical models obeying the Poincaré algebra

$$\{H, B\} = P, \quad \{P, B\} = H, \quad \{H, P\} = 0 \quad [14]$$

Here, H will be the Hamiltonian of the system generating time translations, P is a space-translation

generator, and B the generator of boosts. Ruijsenaars and Schneider began with the ansatz

$$H = \sum_{j=1}^n \cosh p_j \prod_{k \neq j} f(x_j - x_k)$$

$$P = \sum_{j=1}^n \sinh p_j \prod_{k \neq j} f(x_j - x_k)$$

$$B = \sum_{j=1}^n x_j$$

With this ansatz and the canonical Poisson bracket $\{p_i, x_j\} = \delta_{ij}$, the first two Poisson brackets of [14] involving the boost operator B are automatically satisfied. The remaining Poisson bracket is then

$$\begin{aligned} \{H, P\} = & - \sum_{j=1}^n \partial_j \prod_{k \neq j} f^2(x_j - x_k) \\ & - \frac{1}{2} \sum_{j \neq k} \cosh(p_j - p_k) \prod_{l \neq j} f(x_j - x_l) \\ & \times \prod_{m \neq k} f(x_k - x_m) (\partial_j \ln f(x_k - x_j) \\ & + \partial_k \ln f(x_j - x_k)) \end{aligned}$$

and for the independent terms proportional to $\cosh(p_j - p_k)$ to vanish we require that $f'(x)/f(x)$ be odd. This entails that $f(x)$ is either even or odd (Ruijsenaars and Schneider assumed the function even) and in either case $F(x) = f^2(x)$ is even. Supposing that $f(x)$ is so constrained, then the final Poisson bracket is equivalent to the functional equation

$$\{H, P\} = 0 \iff \sum_{j=1}^n \partial_j \prod_{k \neq j} f^2(x_j - x_k) = 0 \quad [15]$$

For $n=3$, eqn [15] takes precisely the form [12] with $F(x) = f^2(x)$. From Theorem 2, the even solutions to this have the form $F(x) = \wp(x) + c$. This was found by Ruijsenaars and Schneider who further showed this function satisfies [15] for all n . The general solution to [15] has recently been established.

Theorem 3 (Byatt-Smith and Braden 2003). *The general even solution of [15] amongst the class of meromorphic functions whose only singularities on the real axis are either a double pole at the origin, or double poles at np (p real, $n \in \mathbb{Z}$) is:*

(i) for all odd n given by the solution of Ruijsenaars and Schneider while

(ii) for even $n \geq 4$, there are in addition to the Ruijsenaars–Schneider solutions the following:

$$F_i(z) = \sqrt{(\wp(z) - e_j)(\wp(z) - e_k)} \quad [16]$$

where i, j, k are a cyclic permutation of 1, 2, 3.

These functions have simple expressions in terms of Weierstrass elliptic functions, theta functions, and the Jacobi elliptic functions (Whittaker and Watson 1927). For example,

$$\begin{aligned} F_1(z) &= \sqrt{(\wp(z) - e_2)(\wp(z) - e_3)} = \frac{\sigma_2(z)\sigma_3(z)}{\sigma^2(z)} \\ &= \frac{\theta_3(v)\theta_4(v)}{\theta_1^2(v)} \frac{\theta_1^2(0)}{4\omega^2\theta_3(0)\theta_4(0)} = b \frac{\operatorname{dn}(u)}{\operatorname{sn}^2(u)} \end{aligned}$$

where

$$\begin{aligned} \sigma_\alpha(z) &= \frac{\sigma(z + \omega_\alpha)}{\sigma(\omega_\alpha)} e^{-z\zeta(\omega_\alpha)} \\ u &= \sqrt{e_1 - e_3}z \end{aligned}$$

$v = z/2\omega$, $b = e_1 - e_3$ with $\omega_1 = \omega$, $\omega_2 = -\omega - \omega'$, and $\omega_3 = \omega'$. For appropriate ranges of z the solutions are real. Their degenerations yield all the even solutions with only a double pole at $x=0$ on the real axis. These degenerations may in fact coincide with the degenerations of the Ruijsenaars–Schneider solution.

Thus far, complete integrability has not been mentioned. The models discovered by Ruijsenaars and Schneider not only exhibited an action of the Poincaré algebra but were completely integrable as well. In particular, Ruijsenaars and Schneider demonstrated the Poisson commutativity for their solutions of the light-cone quantities

$$S_{\pm k} = \sum_{\substack{I \subseteq \{1, 2, \dots, n\} \\ |I|=k}} \exp\left(\pm \sum_{i \in I} p_i\right) \prod_{\substack{i \in I \\ j \notin I}} f(x_i - x_j) \quad [17]$$

Then, $H = (S_1 + S_{-1})/2$ and $P = (S_1 - S_{-1})/2$. (Note the even/oddness of the functions $f(x)$ means that there really are only n functionally independent quantities.) It is an open problem whether the new solutions [16] of Theorem 3 yield integrable systems. We know that these new solutions do not always yield Poisson commuting quantities using the ansatz of Ruijsenaars and Schneider, but as yet one cannot rule out other Poisson commuting conserved quantities.

Quantum Ruijsenaars–Schneider Models

Ruijsenaars later investigated the quantum version of the classical models he and Schneider introduced.

From the outset, he sought operator analogs of the light-cone quantities [17]. He showed that (for $k = 1, \dots, n$)

$$\hat{S}_k = \sum_{\substack{I \subseteq \{1, 2, \dots, n\} \\ |I|=k}} \prod_{\substack{i \in I \\ j \notin I}} h(x_j - x_i)^{1/2} \\ \times \exp \left(-\sqrt{-1} \beta \sum_{i \in I} \partial_i \right) \prod_{\substack{i \in I \\ j \notin I}} h(x_i - x_j)^{1/2}$$

pairwise commute if and only if

$$\sum_{\substack{I \subseteq \{1, 2, \dots, n\} \\ |I|=k}} \left(\prod_{\substack{i \in I \\ j \notin I}} h(x_j - x_i) h(x_i - x_j - i\beta) \right. \\ \left. - \prod_{\substack{i \in I \\ j \notin I}} h(x_i - x_j) h(x_j - x_i - i\beta) \right) = 0 \quad [18]$$

held for all k and $n \geq 1$. Here, β is an arbitrary positive number and the sum is over all subsets with k elements. Observe that upon dividing [18] by β and letting $\beta \rightarrow 0$ this yields [15] with $F(x) = h(x)h(-x)$ when $k = 1$.

Ruijsenaars found a solution to [18] which has subsequently been shown to be unique. The general solution of the functional equation [18] analytic in a neighborhood of the real axis with either a simple pole at the origin or an array of such poles at $n\pi$ on the real axis ($n \in \mathbb{Z}$) is given by

$$h(x) = b \frac{\sigma(x + \nu)}{\sigma(x) \sigma(\nu)} e^{\alpha x} \quad [19]$$

This solution is related to the earlier Ruijsenaars–Schneider solution via

$$\frac{\sigma(x + \nu) \sigma(x - \nu)}{\sigma^2(x) \sigma^2(\nu)} = \wp(\nu) - \wp(x)$$

Geometric Ansatz

We have already encountered the Hamiltonian system [10] corresponding to geodesic motion while discussing Lax pairs. We shall now consider various ansätze with a geometric flavor and their attendant functional equations.

It is known that the Ruijsenaars–Schneider model has the Calogero–Moser system as a scaling limit. Other scaling limits also exist for the Ruijsenaars–Schneider model. In particular, we may consider one in which the Poincaré algebra scales to either the Galilean algebra or a central extension of the Galilean algebra.

Similar to our analysis of the Poincaré algebra, we find that the functions

$$H = \frac{1}{2} \sum_{j=1}^n p_j^2 \prod_{k \neq j} f(x_j - x_k), \\ P = \sum_{j=1}^n p_j \prod_{k \neq j} f(x_j - x_k), \quad B = \sum_{j=1}^n x_j$$

obey the algebra

$$\{H, B\} = P, \quad \{P, B\} = \lambda, \quad \{H, P\} = 0 \quad [20]$$

if and only if $f(x)$ is either an even or odd function satisfying

$$\sum_{j=1}^n \prod_{k \neq j} f(x_j - x_k) = \lambda \quad [21]$$

where λ is a constant. When $\lambda = 0$ this is the Galilean algebra, while $\lambda \neq 0$ is a central extension of the Galilean algebra. Again we are encountering models of the form $H = (1/2) \sum_{j=1}^n g^{jj} p_j^2$ and so dealing with diagonal metrics. We note that if [21] holds for $n = 3$ then it holds for all n ; and if it holds for $n = 4$ then it holds for all “even” n . This type of behavior was already encountered in Theorem 3.

Some particular solutions of [21] are known although the general solution is not known as yet. The odd functions $f(x) = 1/x$ ($\lambda = 0$), $\coth(x)$ ($\lambda = 1$ for n odd and $\lambda = 0$ for n even), $\sqrt{\wp(x) - e_\alpha}$ ($\lambda = 0$) yield solutions for example. Interestingly, in the case of an even number of particles, particular cases of the elliptic Ruijsenaars–Schneider model are in this list.

Diagonal metrics arise in many settings in integrable systems. By taking the ansatz

$$ds^2 = \sum_{i=1}^n \left(\prod_{j \neq i} \Psi(x^i - x^j) \right) (dx^i)^2$$

we may construct and solve a functional equation to show that the potentially nonvanishing curvature components $R_{jik}^i, R_{ijk}^i (k \neq i, j)$, and R_{ijj}^i have

1. $R_{jik}^i = R_{ijk}^i = 0$ ($k \neq i, j$) if and only if $\Psi(x) = \alpha(e^{2bx} - 1)^a$ or αx^a . We may set $\alpha = 1$ by rescaling x .
2. $R_{ijj}^i = (-1)^n b^2$ when $\Psi(x) = (e^{2bx} - 1)$.
3. $R_{ijj}^i = 0$ when $\Psi(x) = x$.

Thus, $\Psi(x) = x$ yields a solution of the Lamé equations. These metrics are of Stäckel form. The rational degenerations of the Galilean models above are given by this theorem. They may be understood as a parabolic limit of Jacobi elliptic coordinates.

Similar techniques may be applied to the more general metric

$$ds^2 = \sum_{i=1}^n \left(\chi_i(x^i) \prod_{j \neq i} \Psi(x^i - x^j) \right) (dx^i)^2$$

to show that $R_{jik}^i = R_{jjk}^i = 0$ ($k \neq i, j$) if and only if $\Psi(x) = \alpha(e^{2bx} - 1)^a$ or αx^a .

Ground-State Factorization

Some years ago, Sutherland and Calogero considered the problem as to when the ground-state wave function of a one-dimensional n -body Schrödinger equation with pairwise interactions would factorize. Thus, the problem is to determine those potentials $v(x)$ for which

$$\left\{ -\frac{\hbar^2}{2} \sum_{i=1}^n \partial_i^2 + \frac{1}{2} \sum_{i \neq j} v(x_i - x_j) - E \right\} \bar{\Psi}(x_1, x_2 \dots x_n) = 0 \quad [22]$$

and where

$$\bar{\Psi}(x_1, x_2 \dots x_n) = \prod_{i < j} \psi(x_i - x_j)$$

It is convenient to set

$$\psi(x_i - x_j) = \exp\left(\frac{1}{\hbar} \int^{x_i - x_j} f(x) dx\right)$$

Substitution now shows

$$\begin{aligned} \frac{\hbar^2}{2} \sum_{i=1}^n \partial_i^2 \bar{\Psi} = & \left\{ \hbar \sum_{i < j} f'(x_i - x_j) + \sum_{i < j} f(x_i - x_j)^2 \right. \\ & + \sum_{i < j < k} [f(x_i - x_j)f(x_i - x_k) \\ & - f(x_i - x_j)f(x_j - x_k) \\ & \left. + f(x_j - x_k)f(x_i - x_k)] \right\} \bar{\Psi} \end{aligned}$$

Comparison with [22] shows that this may be expressed in terms of two-body potentials if and only if we have the functional equation

$$f(a)f(-b) - f(a)f(c) + f(c)f(-b) = G_1(a) + G_1(c) + G_2(-b), \quad a + b + c = 0 \quad [23]$$

Now [23] is not quite the functional equation studied by Sutherland and Calogero. On physical grounds, Sutherland implicitly, and Calogero explicitly, made the "assumption" that f is an odd function. This ensured that the potential was even and so bounded from below; equally it may be

imposed so that $\psi(x_i - x_j) = \psi(x_j - x_i)$ and the ground state describes bosons. With this assumption, one arrives at the functional equation of Sutherland:

$$f(a)f(b) + f(b)f(c) + f(c)f(a) = G(a) + G(b) + G(c) \quad [24]$$

Actually the assumption of f being odd is unnecessary. One can show that there is a bijection between analytic solutions of [23] and analytic solutions of [24] for which $f'(x)$ is even. Upon requiring a potential of the stated form then necessitates f being odd. Whatever, we arrive at the functional equation [24]. This is connected with [12] by

Lemma 4 If $a + b + c = 0$, then

$$\begin{vmatrix} f''(a) & f''(b) & f''(c) \\ f'(a) & f'(b) & f'(c) \\ 1 & 1 & 1 \end{vmatrix} = 0 \quad [25]$$

$$\iff (f(a) + f(b) + f(c))^2 = F(a) + F(b) + F(c) \quad [26]$$

$$\iff f(a)f(b) + f(b)f(c) + f(c)f(a) = G(a) + G(b) + G(c) \quad [27]$$

Now, we may use Theorem 2 to determine those potentials with factorizable ground-state wave functions. We remark that the δ -function potential $a\delta(x)$ of many-body quantum mechanics on the line, which also has a factorizable ground-state wave function, can be viewed as the $\alpha \rightarrow 0$ limit of $-b/\alpha \sinh^2(-x/\alpha + \pi i/3)$ with $\pi a\alpha = 6b$. Thus, all of the known quantum mechanical problems with factorizable ground-state wave function are included in [12].

Baker-Akierzer Functions

Baker-Akierzer functions are one of the foundations of the algebro-geometric or finite-gap integration of integrable systems. These functions may be viewed as an extension of the exponential function to curves of arbitrary genus g . They have essential singularities at various points on the curve and a prescribed asymptotic expansion at these points. The functions may be described in terms of theta functions on the Jacobian of the curve, and suitable meromorphic differentials on the curve. The functions [6] and [19] may be viewed as the Baker-Akhiezer function for a genus-1 curve. Now, just as the exponential function satisfies Cauchy's functional equation one may ask what functional equations (if any) characterize the

Baker–Akiezer function. This is an area of research still ongoing. Theta functions of a general abelian variety are known to satisfy addition formulas with $N=2^g$ terms. It appears Baker–Akiezer functions satisfy a similar functional equation with far fewer terms. Such a characterization of Baker–Akiezer functions, if found, will provide an analogous answer to that of the Riemann–Schottky problem which seeks to describe the Jacobians of curves amongst general abelian varieties.

The functional equations [5], and after suitably symmetrizing [9], are particular cases of the functional equation

$$\sum_{i=0}^N \phi_{3i}(x+y) \begin{vmatrix} \phi_{3i+1}(x) & \phi_{3i+1}(y) \\ \phi_{3i+2}(x) & \phi_{3i+2}(y) \end{vmatrix} = 0 \quad [28]$$

with $N=1$ in the former case and $N=2$ in the latter. In the case $\phi_{3i+2} = \phi'_{3i+1}$, these may be viewed as differentiated forms of

$$\sum_{i=0}^N \phi_{3i}(x+y) \phi_{3i+1}(x) \phi_{3i+1}(y) = 1 \quad [29]$$

For $N=0$, this is Cauchy’s equation characterizing the exponential function and for $N=2$ it is equivalent to [8]. For $N=1$ and $N=2$, Buchstaber and Krichever have shown that “all” the solutions to this equation are the Baker–Akhiezer functions corresponding to algebraic curves of genus 1 and 2, respectively. In general, the Baker–Akhiezer functions for a genus- g curve are known to satisfy [29] for $N=g$. Thus, many of the equations we have encountered are related to Baker–Akhiezer functions. Dubrovin, Fokas, and Santini have shown that Baker–Akhiezer functions for a genus- g curve are related to the functional equation

$$\frac{q(x,y)q(y,z)}{q(x,z)} = r(x,y) - r(z,y) + \sum_{k=1}^g s_k(y) p_k(x,z)$$

Multivariable generalizations of [29] have been sought as a means of characterizing Baker–Akhiezer functions but such a characterization remains unproved as yet.

Topology

Several of the functional equations we have encountered also arise in topology, where the German and Russian schools have powerfully applied functional equations to formal group laws and genera. It is still unclear whether these common threads form part of a greater fabric. A genus is a ring homomorphism

$$\varphi : \Omega \otimes \mathbb{Q} \rightarrow R, \quad \varphi(1) = 1$$

where Ω is the cobordism ring and R an integral domain over \mathbb{Q} . To each even power series $Q(x)$ with $Q(0)=1$, one can associate a genus φ_Q and vice versa (Hirzebruch *et al.* 1992). Defining the odd power series $f(x)=x/Q(x)$ with first term 1 and coefficients in R , the inverse function $g=f^{-1}$ is such that

$$g'(y) = \sum_{n=0}^{\infty} \varphi_Q(\mathbb{CP}^n) y^n$$

The genus corresponding to $Q(x)=x/\tanh(x)$ is known as the L -genus; it takes the value 1 on every even complex projective space. The genus corresponding to $Q(x)=(x/2)/\sinh(x/2)$ is known as the \hat{A} -genus. The so-called (string-inspired) Witten or elliptic genus corresponds to $Q(x)=x/\sigma(x)$. Certain genera may be associated with the index of natural differential operators on the manifold. Thus, the signature of M , $\text{sign}(M)$, is given in terms of the de Rham differential d and its adjoint d^* ,

$$\text{ind}(d+d^*) = \text{sign}(M) = \left(\prod_{j=0}^{2n} \frac{x_j}{\tanh(x_j)} \right) [M]$$

with variants for the \hat{A} -genus and elliptic genus. Further, when a compact topological group acts on the manifold, Atiyah and Bott showed how these indices may be determined from the fixed point sets of the action.

Now, functional equations arise naturally in this context when seeking genera with special properties. Novikov’s school has shown, for example, that the genera associated with the index theorems of known elliptic operators arise as solutions of functional equations which are particular examples of [5]. Similarly, one may seek the following property of a genus φ : for the fiber bundle $p:E \xrightarrow{F} B$ with smooth fiber and base, one has that

$$\varphi(E) = \varphi(F) \cdot \varphi(B)$$

Such a genus is said to be strictly multiplicative. It may be shown that a genus is strictly multiplicative in bundles with fiber \mathbb{CP}^{n-1} if and only if

$$\sum_{j=1}^n \prod_{k \neq j} \frac{1}{f(x_j - x_k)} = \lambda \quad [30]$$

which is essentially [21]. Following the remarks of that equation, a genus φ is strictly multiplicative for all fiber bundles with fibers \mathbb{CP}^{n-1} if and only if it is strictly multiplicative for all fiber bundles with fiber \mathbb{CP}^2 , in which case the genus is the L -genus. If, on the other hand, we only demand strict multiplicativity for all fiber bundles with fibers \mathbb{CP}^{2k-1} , then this is equivalent to requiring it to hold for all fiber bundles with fiber \mathbb{CP}^3 , in which case the genus is an elliptic

genus. That the same functional equations arise in both the integrable systems and topological settings may reflect something deeper. String theory physics, for example, allows some topology changes such as flops, and physical quantities such as the partition function should reflect this invariance; invariance under classical flops characterizes the elliptic genus. In addition, connections have been made between the complex cobordism ring and conformal field theory.

Other Areas

The constraints placed on this review have meant that several further applications of functional equations and integrable systems can only be noted. Using an ansatz together with functional equations, Wojciechowski gives an analog of the Bäcklund transformation for integrable many-body systems. Similarly, Inozemtsev constructs generalizations of the Calogero–Moser models, while this route was used to construct new solutions to the Witten–Dijkgraaf–Verlinde–Verlinde (WDVV) equations by Braden, Marshakov, Mironov, and Morozov. In the quantum regime, Gutkin derived and solved several functional relations by requiring a nondiffractive potential, while functional equations have been used to construct R -operators, solutions of the quantum Yang–Baxter equation on a function space.

See also: Calogero–Moser–Sutherland Systems of Nonrelativistic and Relativistic Type; Classical r -matrices, Lie Bialgebras, and Poisson Lie Groups; Cohomology Theories; Eigenfunctions of Quantum Completely Integrable Systems; Integrability and Quantum Field Theory; Integrable Systems and Algebraic Geometry; Integrable Systems: Overview; Lie Groups: General Theory; Quantum Calogero–Moser Systems; Toda Lattices; WDVV Equations and Frobenius Manifolds.

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Functional Integration in Quantum Physics

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The Domain of Integration

Functional integration is integration over function spaces, that is, the variable of integration is a function f with values in a D -dimensional manifold:

$$f : U \longrightarrow \mathbb{M}^D \quad [1]$$

Generically a space of functions is an infinite-dimensional space. Our understanding of infinite-dimensional spaces has progressed significantly during the twentieth century, and we can formulate functional integration in its proper setting.

Let \mathcal{F} be the domain of integration, and $f \in \mathcal{F}$ the variable of integration. If the domain of f is a subset U of \mathbb{R} , the functional integral is called a path integral; if U is of dimension higher than 1 (e.g., spacetime), \mathcal{F} is often called a space of histories.

The information necessary for defining a domain of integration includes

- the domain and the range of the variable of integration f ,
- the analytical properties of f , and
- possibly additional information, such as requirements on the values of f on its boundary.

Examples of variables of integration f in [1]

The domain U of f may be a time interval, a scale range, or any parameter. The range \mathbb{M}^D of f may be a group manifold, a Riemannian manifold, a symplectic manifold, a multiply-connected space, etc., or simply \mathbb{R}^D . The domain of integration \mathcal{F} may be a space of pointed paths, for example,

$$x := T \longrightarrow \mathbb{M}^D, \quad T = [t_a, t_b] \quad [2]$$

$$x(t_b) = x_b \in \mathbb{M}^D \quad \text{for all } x \in \mathcal{F}$$

The paths x may be continuous (e.g., Brownian paths), or may have square integrable derivatives; \mathcal{F} is then an $L^{2,1}$ space (e.g., quantum physics).

$$\int_T dt |\dot{x}(t)|^2 < \infty, \quad x \in \mathcal{F} \quad [3]$$

Given a domain of integration \mathcal{F} , one needs to select a volume element appropriate to \mathcal{F} . This is a challenge which has been met in a number of cases

(Cartier and DeWitt-Morette 2006). Examples are given below. Given a volume element, one can then characterize the functionals F on \mathcal{F} integrable with respect to the chosen volume element.

Two Basic Techniques

The two most useful techniques for computing integrals are change of variable of integration and integration by parts. They follow from fundamental properties that apply to functional integrals as well as to ordinary integrals. Let us recall them in the context of ordinary integrals.

Let f and g be functions on \mathbb{R} of compact support. Let I stand for integration

$$I(f) = \int_{\mathbb{R}} dx f(x), \quad x \in \mathbb{R}$$

and D for derivation of f with respect to x ,

$$(Df)(x) = \frac{d}{dx} f(x)$$

The fundamental rule

$$DI = 0 \implies 0 = \frac{d}{dx} \int_{\mathbb{R}} dx f(x) \quad [4]$$

The functional $I(f)$ is invariant under a change of variable of integration.

Another fundamental rule is $ID = 0$:

$$\begin{aligned} ID = 0 \implies 0 &= \int d(f(x)g(x)) \\ &= \int df(x) \cdot g(x) + \int dg(x) \cdot f(x) \end{aligned} \quad [5]$$

The fundamental rules [4] and [5] apply to functional integration. The derivation D can be either a functional derivative or a Lie derivative defined as follows. Let \mathbb{K} be the reals \mathbb{R} or the complex \mathbb{C} , let f be a differentiable functional on a Banach space \mathbb{X}

$$f : U \subset \mathbb{X} \longrightarrow \mathbb{K} \quad [6]$$

The functional derivative $Df|_{x_0}$ of f at x_0 is defined by the equation

$$f(x_0 + h) - f(x_0) = Df|_{x_0} h + R(h) \quad [7]$$

with the norm $\|R(h)\|$ of order less than the norm $\|h\|$.

The Lie derivative \mathcal{L}_V along the vector field V is conceptually intuitive and of practical interest: an infinite-dimensional space \mathbb{X} of paths x is not an intuitive concept, but a one-parameter family of

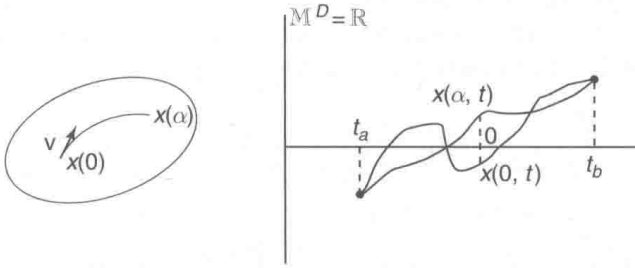


Figure 1 A one-parameter family of paths with fixed endpoints.

paths $\{x(\alpha)\} \in \mathbb{X}$, with $\alpha \in [0, 1]$, is a convenient tool for dealing with \mathbb{X} :

$$\begin{aligned} x(\alpha) : T &\rightarrow \mathbb{M}^D \\ x(\alpha, t) &:= (x(\alpha))(t) \in \mathbb{M}^D \end{aligned} \quad [8]$$

Set $x(0) = x_0$. A differentiable family $\{x(\alpha)\}$ defines a vector field $V(x_0)$ along the path x_0 (see **Figure 1**):

$$\begin{aligned} V(x_0) &:= \left. \frac{d}{d\alpha} x(\alpha) \right|_{\alpha=0} \\ V(x_0(t)) &= \left. \frac{\partial}{\partial \alpha} x(\alpha, t) \right|_{\alpha=0} \end{aligned} \quad [9]$$

The functional vector field V on the tangent bundle of \mathbb{X} defines a group of transformations on \mathbb{X} , and a Lie derivative \mathcal{L}_V of tensor fields on \mathbb{X} .

The Lie derivative \mathcal{L}_V obeys the Cartan (Elie and Henri) equation

$$\mathcal{L}_V = d\iota_V + \iota_V d \quad [10]$$

where d is the exterior differential and ι_V is the interior product, defined as usual on Banach spaces.

Remark (Berezin integrals). To show the power of the rules [4] and [5], we can mention that they provide Berezin rules of integration over Grassmann variables (Cartier and DeWitt-Morette 2006).

Path Integrals and Quantum Dynamics

The history of path integrals in quantum physics did not begin with the definitions of domain of integration, volume elements, etc. It began with the Ph.D. thesis of R P Feynman in 1942. Feynman expressed the time evolution of a system as the limit $N = \infty$ of the following N -tuple integral:

$$\begin{aligned} (x_t|x_a) &= \lim_{N \rightarrow \infty} \int \cdots \int (x_t|x_N) dx_N (x_N|x_{N-1}) \\ &\quad \times dx_{N-1} \cdots (x_2|x_1) dx_1 (x_1|x_0) \end{aligned} \quad [11]$$

where the time interval $T = [t, 0]$ has been replaced by N of its points $\{t_i\}$, $1 \leq i \leq N$:

$$t_0 < t_1 < \cdots < t_N < t \quad [12]$$

and the path $x : T \rightarrow \mathbb{R}^D$ is replaced by N of its values

$$x_i := x(t_i) \quad [13]$$

Dirac (1933) had shown that $(x_t|x_0)$ defines the exponential of a quantum function S_Q , by

$$\exp(iS_Q(x_t, x_0, t)/\hbar) := (x_t|x_0) \quad [14]$$

such that the real part of S_Q is the classical action function (a.k.a. Hamilton's principal function; further studies have shown that the correct statement is: the real part is the classical action, up to order \hbar), and the imaginary part of S_Q is of order \hbar , the normalized Planck constant

$$\hbar = h/2\pi \quad [15]$$

Feynman remarked that for a system with Lagrangian L the short-time probability amplitude $(x_{t+\delta t}|x_t)$ is "often equal to

$$A^{-1} \exp\left(i \delta t L\left(\frac{x_{t+\delta t} - x_t}{\delta t}, x_{t+\delta t}\right)/\hbar\right) \quad [16]$$

within a normalizing constant A as the limit δt approaches zero." The absolute value of A can be obtained from a unitary requirement (Morette 1951).

Feynman expressed the finite probability amplitude as a path integral, limit of the discretized expression [11]

$$(x_t|x_0) = \int \mathcal{D}x \exp(iS(x)/\hbar) \quad [17]$$

where $S(x)$ is the action functional

$$S(x) = \int_{t_0}^t ds L(\dot{x}(s), x(s)) \quad [18]$$

The undefined symbol $\mathcal{D}x$ is a "volume element" on the space of paths, corresponding to the infinite product of the normalization constant A^{-1} .

The issues raised by the path integral [17] are

- the definition of the volume element $\mathcal{D}x$; and
- a method for computing [17] for a given action functional S .

The explicit calculation of the limit [11] of an N -tuple integral when $N = \infty$ is a Herculean task of very limited use. But two other methods of wide applications, leaving the volume element $\mathcal{D}x$ as a heuristic symbol, have vindicated the power of functional integration: the diagram technique and the semiclassical expansions.

Feynman devised practical rules for computing asymptotic expansions of path integrals, order by order in perturbation theory. The rules are depicted by graphs, known as the Feynman diagrams ('t Hooft and Veltmann 1973). Feynman's first explicit nontrivial calculation was the Lamb shift. It earned him the Nobel prize in 1965 (Feynman 1966). The diagram technique is widely used in quantum mechanics and quantum field theory. The time ordering provided by the time parameter in quantum mechanics becomes, in quantum field theory, a chronological ordering dictated by light cones.

Another explicit calculation of a path integral [17] uses the Taylor expansion of the action functional $S(x)$ around one of its values. It is known as the background method (DeWitt 2004). It is called a semiclassical WKB approximation when one expands around an extremum $S(x_{cl})$ where x_{cl} is a solution of the Euler–Lagrange equation $S'(x_{cl})=0$ (Wenzel 1926, Kramers 1927, Brillouin 1926).

Introduced in 1951 (Morette (1951)) semiclassical approximations are now the subject of a rich literature reviewed briefly below.

Gaussian Volume Elements

A lesson from Gaussians on \mathbb{R}^D suggests a definition of volume elements on infinite-dimensional Banach spaces \mathbb{X} . Let

$$I_D(a) := \int_{\mathbb{R}^D} dx \exp\left(-\frac{\pi}{a}|x|^2\right) \quad \text{for } a > 0 \quad [19]$$

$$dx = dx^1 \cdots dx^D \quad \text{and} \quad |x|^2 = \sum_{j=1}^D (x^j)^2 = \delta_{ij} x^i x^j$$

An elementary calculation gives $I_D(a) = a^{D/2}$. Therefore, when $D = \infty$,

$$I_\infty(a) = \begin{cases} 0 & \text{if } 0 < a < 1 \\ 1 & \text{if } a = 1 \\ \infty & \text{if } 1 < a \end{cases} \quad [20]$$

This is clearly an unsatisfactory situation, but it can be corrected by introducing a dimensionless volume element:

$$\mathcal{D}_a x := \frac{1}{a^{D/2}} dx^1 \cdots dx^D \quad [21]$$

The volume element $\mathcal{D}_a x$ can be defined by the integral

$$\begin{aligned} \int_{\mathbb{R}^D} \mathcal{D}_a x \exp\left(-\frac{\pi}{a}|x|^2 - 2\pi i \langle x', x \rangle\right) \\ := \exp\left(-a\pi |x'|^2\right) \end{aligned} \quad [22]$$

where x' is in the dual \mathbb{R}_D of \mathbb{R}^D . Equation [22] suggests the following generalization of Gaussians on \mathbb{R}^D to Gaussians on a Banach space \mathbb{X} :

$$\begin{aligned} \int_{\mathbb{X}} \mathcal{D}_{s,Q} x \exp\left(-\frac{\pi}{s} Q(x)\right) \exp(-2\pi i \langle x', x \rangle) \\ := \exp(-s\pi W(x')) \end{aligned} \quad [23]$$

where $s \in \{1, i\}$, $Q(x)$ is a quadratic form on \mathbb{X} (see condition on Q below). $W(x')$ is a quadratic form on the dual \mathbb{X}' of \mathbb{X} , inverse of $Q(x)$ in the following sense. Set

$$Q(x) = \langle Dx, x \rangle \quad \text{and} \quad W(x') = \langle x', Gx' \rangle \quad [24]$$

where \langle, \rangle is a duality product, for example, the product of $x \in \mathbb{X}$ and $Dx \in \mathbb{X}'$; then

$$DG = 1_{\mathbb{X}'}, \quad GD = 1_{\mathbb{X}} \quad [25]$$

Equation [23] defines a Gaussian volume element $d\Gamma$ by its Fourier transform

$$\begin{aligned} \mathcal{F}\Gamma_{s,Q}(x') &:= \int_{\mathbb{X}} d\Gamma_{s,Q}(x) \exp(-2\pi i \langle x', x \rangle) \\ &:= \exp(-s\pi W(x')) \end{aligned} \quad [26]$$

where the Gaussian volume element

$$d\Gamma_{s,Q}(x) \stackrel{\text{def}}{=} \mathcal{D}_{s,Q}(x) \exp\left(-\frac{\pi}{s} Q(x)\right) \quad [27]$$

This is a qualified equality valid upon integration.

The definition of the Gaussian volume element by its Fourier transform $\mathcal{F}\Gamma$ is valid for $s=1$ (Wiener integral) when $Q(x) > 0$; it is valid for $s=i$ (Feynman integral) when $\text{Re} Q(x) > 0$.

Remark Volume elements were introduced with the notation such as dx ; later they were identified with forms such as $\omega = dx$. In [26] we omit d on the left-hand side (LHS) for visual clarity.

Example (diagram expansion). The following integrals follow readily (Cartier and DeWitt-Morette 2006) from the definition [26]. Let x' be in the dual \mathbb{X}' of \mathbb{X} ,

$$\int_{\mathbb{X}} d\Gamma_{s,Q}(x) \langle x', x \rangle^{2n+1} = 0 \quad [28]$$

$$\int_{\mathbb{X}} d\Gamma_{s,Q}(x) \langle x', x \rangle^{2n} = \frac{2n!}{2^n n!} \left(\frac{s}{2\pi}\right)^n W(x')^n \quad [29]$$

$$\begin{aligned} \int_{\mathbb{X}} d\Gamma_{s,Q}(x) \langle x'_1, x \rangle \cdots \langle x'_{2n}, x \rangle \\ = \left(\frac{s}{2\pi}\right)^n \sum W(x'_{i_1}, x'_{i_2}) \cdots W(x'_{i_{2n-1}}, x'_{i_{2n}}) \end{aligned} \quad [30]$$

where \sum is a sum without repetitions of identical terms.

For instance when $n=1$, eqn [30] reads

$$\int_X d\Gamma_{s,Q}(x) \langle x'_1, x \rangle \langle x'_2, x \rangle = \frac{s}{2\pi} W(x'_1, x'_2) \quad [31]$$

$W(x'_1, x'_2)$ is called the two-point function (a.k.a. the propagator). In a diagram it stands for a line from x'_1 to x'_2 .

Feynman diagrams represent Gaussian integrals of polynomials.

For instance when $n=2$, the diagram representation of [30] is the sum of three terms,

$$W(x'_1, x'_2) W(x'_3, x'_4) + W(x'_1, x'_3) W(x'_2, x'_4) + W(x'_1, x'_4) W(x'_2, x'_3)$$

Example (Linear maps). Linear maps on \mathbb{R}^D are limited to $L: x \rightarrow Ax$, where A is a $D \times D$ constant matrix. Linear maps on a Banach space \mathbb{X} offer many possibilities:

(i) Projections. For example, let $x: T \rightarrow \mathbb{R}$ and

$$L: x \in \mathbb{X} \rightarrow \{x(t_1), x(t_2), \dots, x(t_n)\} \in \mathbb{R}^n \quad [32]$$

This projection is a discretization of the path, useful in particular in numerical calculations of path integrals. Equation [32] is unambiguous, whereas the limit of the discretized expression [11] is ill-defined.

(ii) Liouville decomposition. For example, let D be a second-order differential operator on a space of paths $x: [t_a, t_b] \rightarrow \mathbb{M}^D$ vanishing on the boundary, $x(t_a) = 0, x(t_b) = 0$. Let $\{\varphi_k\}$ be a complete, orthogonal set of eigenfunctions of D , then the decomposition of x into the basis $\{\varphi_k\}$,

$$x^\alpha(t) = \sum_{k=1}^{\infty} u^\alpha \psi_k^\alpha(t) \quad [33]$$

is a linear map

$$L: x \in \mathbb{X} \rightarrow \{u^1, \dots, u^\infty\} \in \mathbb{R}^\infty$$

It is useful in particular for diagonalizing (see, e.g., [107]) the Green function G of D [25] (a.k.a. the covariance in a Gaussian integral [24], or the two-point function in [31]).

(iii) Volterra maps. For example, let $L: \mathbb{X} \rightarrow \mathbb{Y}$ by

$$y(t) = \int_T ds \theta(t-s) x(s) \\ \theta(t-s) = 1 \quad \text{for } s < t, 0 \text{ otherwise} \quad [34]$$

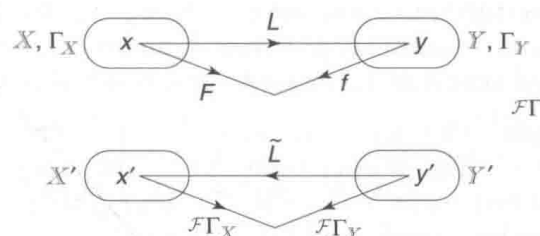


Figure 2 Linear maps. (Published with permission by Elsevier, North Holland.)

Let \mathbb{X} be the space of square-integrable functions on T and \mathbb{Y} be an $L^{2,1}$ space (square-integrable function for which the first derivative is also square integrable) then L maps the canonical quadratic form on \mathbb{X} into the canonical quadratic form on \mathbb{Y} , hence the canonical Gaussian on \mathbb{X} into the canonical Gaussian on \mathbb{Y} . The identity mapping i from \mathbb{Y} into the space \mathcal{C} of continuous functions maps the canonical Gaussian on \mathbb{Y} into the Wiener Gaussian on \mathcal{C} (DeWitt-Morette *et al.* 1979).

The linear maps [32]–[34] and their obvious generalizations have been used for computing explicitly many functional integrals (see Figure 2). The basic formula reads

$$\int_X d\Gamma_X(x) F(x) = \int_Y d\Gamma_Y(y) f(y), \quad F = f \circ L \quad [35]$$

where the Fourier transform $\mathcal{F}\Gamma$ is given by

$$\mathcal{F}\Gamma_Y = \mathcal{F}\Gamma_X \circ \tilde{L} \quad [36]$$

\tilde{L} is the transpose of the linear map L defined by

$$\langle \tilde{L}y', x \rangle = \langle y', Lx \rangle \quad [37]$$

Computing $\mathcal{F}\Gamma_Y$ does not require any calculation. It can be read off eqn [36]. Computing $d\Gamma_Y$ is easy in a number of cases such as the following:

1. \mathbb{Y} is finite-dimensional. In other words [35] is a cylindrical integral. Then

$$d\Gamma_Y(y) = dy^1 \cdots dy^D (\det Q_{ij})^{1/2} \\ \times \exp\left(-\frac{\pi}{s} Q(y)\right) \quad [38]$$

where $Q(y)$ is an abbreviation of

$$Q_Y(y) = Q_{Yij} y^i y^j \quad [39]$$

its inverse $W_{Y'}(y')$ in the sense of [24]–[25] is

$$W_{Y'}(y') = W_{Y'ij} y'^i y'^j \quad [40]$$

that is given by [36]:

$$W_{Y'}(y') = W_{X'} \circ \tilde{L} \quad [41]$$

$W_{X'}$ is the quadratic form defining Γ_X by [26]. When D is small, say less than 4, and this is not an unusual situation, it is easy to compute [38].

Example (Wiener Gaussians and Brownian motion). The Wiener Gaussian on the space $\mathcal{P}_a\mathbb{R}$ of pointed paths $x: T \rightarrow \mathbb{R}$, $T = [t_a, t_b]$, $x(t_a) = 0$ is defined by its variance [26]:

$$W(x') := \int_T dx'(t') \int_T dx'(s) \inf(t, s) \quad [42]$$

Let \mathbb{Y} be the Wiener differential space consisting of the differences of two consecutive values of x on the n -discretized time interval. The space \mathbb{Y} is finite dimensional,

$$L: \mathbb{X} \rightarrow \mathbb{Y}$$

$$\text{by } y^j = x(t_{j+1}) - x(t_j) = \langle \delta_{t_{j+1}} - \delta_{t_j}, x \rangle$$

It follows from [37] that

$$\tilde{L}y' = \sum_j y'_j (\delta_{t_{j+1}} - \delta_{t_j})$$

and

$$\begin{aligned} d\Gamma_Y(\Delta x) &= dy^1 \cdots dy^n \frac{1}{\prod_{j=1}^n (s\Delta t_j)^{1/2}} \\ &\times \exp\left(-\frac{\pi}{s} \sum_j \frac{(\Delta x_j)^2}{\Delta t_j}\right) \end{aligned} \quad [43]$$

where $\Delta t_j := t_{j+1} - t_j$ and $\Delta x_j := x(t_{j+1}) - x(t_j)$.

When $s=1$ the Gaussian Γ_Y defines the distribution of a Brownian path. The Gaussian Γ_X of covariance $\inf(t, s)$ is the Wiener measure. \square

2. In semiclassical approximations, \mathcal{Q}_X is the Hessian (second variation) of an action functional \mathcal{S} :

$$\begin{aligned} \mathcal{Q}_X(h) &= \left. \frac{d^2}{d\alpha^2} \mathcal{S}(x(\alpha)) \right|_{\alpha=0} \\ \text{with } h &= \left. \frac{\partial}{\partial \alpha} x(\alpha) \right|_{\alpha=0} \end{aligned} \quad [44]$$

where $\{x(\alpha)\}$ is a one-parameter family of paths [8]. The Jacobi field technology (the Jacobi operator is defined by [103]; a Jacobi field is a solution of [102]) yields the inverse of $W_{Y'}$ and its determinants (Cartier and DeWitt-Morette 2006); they have been worked out for a variety of boundary conditions on classical paths.

Volume Elements Other than Gaussian

The definition [26]–[27] of Gaussian volume elements is a particular case of volume elements on a Banach space Φ defined by

$$\int_{\Phi} \mathcal{D}_{\Theta, Z} \varphi \cdot \Theta(\varphi, J) := Z(J) \quad [45]$$

for φ in Φ , and J in the dual Φ' of Φ . The volume element $\mathcal{D}_{\Theta, Z}$ is defined by two continuous bounded functionals

$$\Theta: \Phi \times \Phi' \rightarrow \mathbb{C} \quad \text{and} \quad Z: \Phi' \rightarrow \mathbb{C} \quad [46]$$

In quantum field theory, φ is a field and J is a source. The functional $Z(J)$ is then the Schwinger generating functional for the n -point functions. An axiomatic and applications of functional integrals on Φ with volume elements $\mathcal{D}_{\Theta, Z}$ can be found in (Cartier and DeWitt-Morette (1993)).

Example (Poisson volume elements) (Cartier and DeWitt-Morette (2006) and Collins (1997)). A Poisson random variable is a random variable N taking values in the set \mathbb{N} of non-negative integers such that the probability p_n that $N=n$ is

$$p_n := \Pr(N=n) := \exp(-\lambda) \frac{\lambda^n}{n!}, \quad \lambda \geq 0 \quad [47]$$

Thanks to the normalizing constant $\exp(-\lambda)$, $\sum_{n=0}^{\infty} p_n = 1$. The parameter λ is the mean value of N :

$$\langle N \rangle = \lambda \quad [48]$$

A record of fortuitous events occurring at random times $t_0 < T_1 < T_2 \cdots$ can consist either of the number $N(t)$ of events occurring at times less than or equal to t , or of the waiting times

$$W_k = T_k - T_{k-1} \quad [49]$$

between two consecutive events.

When the waiting times are stochastically independent and when

$$\Pr(t < W_k < t + dt) = p_a(t) dt \quad [50]$$

$$p_a(t) = a \exp(-at), \quad t > 0 \quad [51]$$

the record is a Poisson random variable. It is related to the number of events $N(t)$ as follows.

Let T be a finite time interval $[t', t'']$, and

$$N_T = N(t'') - N(t') \quad [52]$$

the number of events during T . The random variable N_T follows a Poisson law [47] with mean value

$$\lambda_a(T) = a(t'' - t') \quad [53]$$

For mutually disjoint time intervals $T^{(1)}, T^{(2)}, \dots$ the random variables $N_{T^{(1)}}, N_{T^{(2)}}, \dots$ are stochastically independent.

Whereas the parameter λ must be real non-negative, the parameter a can be pure imaginary; therefore, Poisson processes defined by waiting

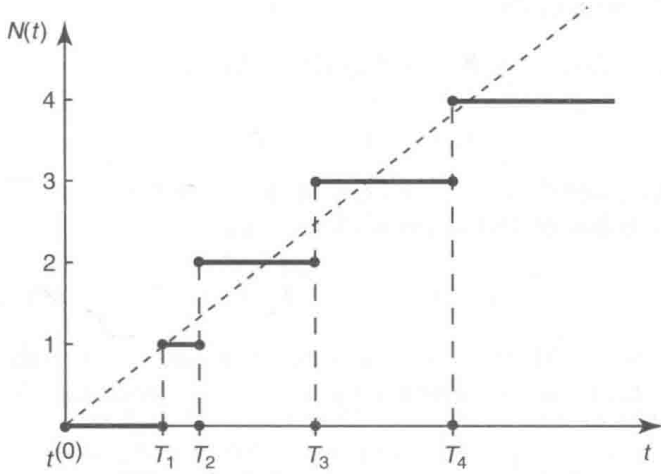


Figure 3 A Poisson path in \mathbb{X}_4 .

times can be used in quantum physics as well as in probability. When a is real, it is called the decay constant because its physical dimension is $[\text{time}]^{-1}$.

A Poisson path $x \in \mathbb{X}_n$ is characterized by n jumps and the jump times during a given time interval $T = [t_a, t_b]$ (Figure 3 illustrates a Poisson path in \mathbb{X}_4). The space \mathbb{X} of Poisson paths is the union of all \mathbb{X}_n :

$$\mathbb{X} = \bigcup \mathbb{X}_n \quad [54]$$

One can define a volume element $\mathcal{D}_{a,T}$ on \mathbb{X} by its Fourier transform:

$$\int_{\mathbb{X}} \mathcal{D}_{a,T} x \cdot \exp(i\langle x, f \rangle) := \exp\left(\int_T dt a e^{if(t)}\right) \quad [55]$$

Here a path $x \in \mathbb{X}_n$, characterized by n jump times T_1, \dots, T_n , is represented by the sum

$$\delta_{T_1} + \dots + \delta_{T_n}$$

Hence

$$\langle x, f \rangle = f(T_1) + \dots + f(T_n) \quad [56]$$

The dimensionless volume element on T is

$$dv(t) = a dt$$

Therefore,

$$\text{vol}(T) = aT, \quad T = t_b - T_a$$

$$\text{vol}(\mathbb{X}_n) = a^n T^n / n! \quad [57]$$

$$\text{vol}(\mathbb{X}) = \exp(\text{vol}(T)) \quad [58]$$

and it makes sense to write formally

$$\mathbb{X} = \exp T$$

It can be proved that the volume element $\mathcal{D}_{a,T} x$ is a measure, in the technical sense of the word (Cartier and DeWitt-Morette 2006).

Functional integration on spaces of Poisson paths have been used extensively in solutions of Klein-Gordon equations, the telegrapher equation and the Dirac equation (Cartier and DeWitt-Morette 2006).

Other volume elements of interest in quantum physics include (LaChapelle 2004):

- gamma volume elements, which are to gamma probability distributions what Gaussian volume elements are to Gaussian probability distributions; and
- Hermite volume elements convenient for integrating Wick-ordered polynomials.

A Dirac “ δ -function” is formally the limit of a Gaussian integral. Formally, one can introduce a Dirac functional volume element as the limit of a Gaussian volume element.

The Koszul Formula

There are several roadblocks on the road from finite to infinite-dimensional spaces. For instance, a volume in a D -dimensional space is a top-differential form, that is, a D -form. There is no top-form in an infinite-dimensional space – neither on Grassmann manifolds since Grassmann forms are totally symmetric tensors. A D -form in \mathbb{R}^D has only one strict component and is equivalent to a scalar density of weight 1, but scalar densities of weight 1 do not form an algebra.

For these reasons, volume elements have so far been defined by integrals [26], [27], [43], and [55]. Short of giving an explicit expression for their differential forms, one can require them to satisfy the Koszul formula

$$\mathcal{L}_X \omega = \text{Div}(X) \omega \quad [59]$$

where ω is a volume element on a Banach space \mathbb{X} , X a vector field generating a group of transformations on \mathbb{X} , \mathcal{L}_X the Lie derivative defined by X , and $\text{Div}(X)$ the standard generalization of $\text{div}(\text{ergence})$ on finite-dimensional spaces (see, e.g., Cartier and DeWitt-Morette (2006) for the explicit expression of divergences on Riemannian, symplectic, Grassmann manifolds). The Koszul formula dictates how a volume element changes under a group of transformations.

It often happens that an object cannot be defined *per se*, but that it is sufficient to define its variation. For example, one does not define potentials, but potential differences; the ratio of infinite-dimensional determinants can be defined without defining each determinant; the work of Wiener on “differential-spaces,” which is a landmark in functional integration, is based

on differences between two consecutive values of a function, etc. Similarly, the Koszul formula does not define ω but gives its variation $\mathcal{L}_X\omega$.

The Operator Formalism of Quantum Physics

Functional integrals can be used to represent operator matrix elements, and solutions of the Schrödinger equation.

1. Matrix elements of operators on Hilbert spaces. Symbolically,

$$\langle \beta | \exp(-iHt/\hbar) | \alpha \rangle = \int_{X_{\alpha\beta}} \mathcal{D}x \exp(iS(x)/\hbar) \quad [60]$$

The domain of integration $X_{\alpha\beta}$ is a space of paths x on $[t, 0]$ satisfying initial conditions that characterize the quantum state α , and final conditions that characterize the quantum state β . The action functional S yields the Hamiltonian H .

A key property of path integrals is their representations of matrix elements of time-ordered operators. The path parameter (time, scale, or any other parameter) provides the operator ordering [11]. A simple example is the two-point function of the Wiener measure [42]:

$$\int_X d\Gamma(x) x(t)x(s) = \inf(t, s) \quad [61]$$

The function integral orders the time, that is, the argument of the variable of integration. In quantum field theory, time ordering becomes a chronological ordering dictated by light cones.

2. Schrödinger equation and other parabolic equations (Cartier and DeWitt-Morette 2006).

The following theorem provides the mathematical underpinning for a great variety of functional integrals. It also provides a construction of functional integrals, which begins with the symmetries of a given physical system rather than its action functional. The theorem consists of two parts: the definition of a functional integral, and the partial differential equation satisfied by the value of the functional integral, as a function of a set of parameters.

Given a manifold M , consider the contractible space \mathcal{P}_0M of pointed $L^{2,1}$ paths over $T = [t_a, t_b]$:

$$\begin{aligned} x : T \rightarrow M, \quad \text{e.g., } x(t_b) = x_b, \\ \text{i.e., } x \in \mathcal{P}_0M \end{aligned} \quad [62]$$

Given $D+1$ vector field Y , $\{X_{(\alpha)}\}$, generators of group of transformations on M , define a map

$$P : \mathcal{P}_0\mathbb{R}^D \rightarrow \mathcal{P}_bM \quad \text{by } z \rightarrow x \quad [63]$$

explicitly

$$dx(t, z) = X_{(\alpha)}(x(t, z))dz^\alpha + Y(x(t, z))dt \quad [64]$$

$$x(t_b, z) = x_b, \quad z(t_b) = 0 \quad [65]$$

In general, the vector fields do not commute and the solution of [64]–[65] is of the form

$$x(t, z) = x_b \cdot \Sigma(t, z) \quad [66]$$

where $\Sigma(t, z)$ is an element of a group of right actions on M , defined by the $D+1$ generators Y , $\{X_{(\alpha)}\}$:

$$x_b \cdot \Sigma(t+t', z \times z') = x_b \cdot \Sigma(t, z) \cdot \Sigma(t', z')$$

The path z defined on $[t_a, t]$ is followed by the path z' on $[t, t']$.

Consider the following functional integral over $\mathcal{P}_0\mathbb{R}^D$ of a functional of paths on \mathcal{P}_bM :

$$\begin{aligned} (U_T\phi)(x_b) &:= \int_{\mathcal{P}_0\mathbb{R}^D} \mathcal{D}_s z \exp\left(-\frac{\pi}{s} Q(z)\right) \\ &\times \phi\left(x_b \cdot \Sigma(t, z)\right) \end{aligned} \quad [67]$$

where

$$Q(z) = \int_T dt \, h_{\alpha\beta} \dot{z}^\alpha(t) \dot{z}^\beta(t) \quad [68]$$

The functional $(U_T\phi)$ at x_b is a function $\Psi(T, x_b)$. It is a solution of the generalized Schrödinger equation,

$$\frac{\partial \Psi}{\partial T} = \frac{s}{\pi} h^{\alpha\beta} \mathcal{L}_{X_{(\alpha)}} \mathcal{L}_{X_{(\beta)}} \Psi + \mathcal{L}_Y \Psi \quad [69]$$

This equation is valid on manifolds M (e.g., frame bundles, $U(N)$ bundles, multiply connected spaces, symplectic manifold phase space) in arbitrary systems of coordinates.

Example (Polar coordinates on \mathbb{R}^D). Let us abbreviate $z^\alpha(t)$ to z^α , $x^1(t)$ to r , and $x^2(t)$ to θ . It follows from

$$z^1 = r \cos \theta, \quad z^2 = r \sin \theta \quad [70]$$

that

$$\begin{cases} dr = \cos \theta \cdot dz^1 + \sin \theta \cdot dz^2 \\ \quad =: X_{(1)}^1 dz^1 + X_{(2)}^1 dz^2 \\ d\theta = -\frac{\sin \theta}{r} dz^1 + \frac{\cos \theta}{r} dz^2 \\ \quad =: X_{(1)}^2 dz^1 + X_{(2)}^2 dz^2 \end{cases} \quad [71]$$

The dynamical vector fields are, therefore,

$$X_{(1)} = \cos \theta \frac{\partial}{\partial r} - \frac{\sin \theta}{r} \frac{\partial}{\partial \theta} \quad [72]$$

$$X_{(2)} = \sin \theta \frac{\partial}{\partial r} + \frac{\cos \theta}{r} \frac{\partial}{\partial \theta} \quad [73]$$

Here $h^{\alpha\beta} = \delta^{\alpha\beta}$ and eqn [69] reads

$$\frac{\partial \Psi}{\partial t} = \frac{s}{4\pi} \left(\frac{\partial^2}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} + \frac{1}{r} \frac{\partial}{\partial r} \right) \Psi \quad [74]$$

This example is trivial because $x(t, z)$ is not a functional of z but a function of $z(t)$ given by [70]. In the following example, $x(t, z)$ is a functional of z .

Example (Paths with values on a Riemannian manifold (M^D, g)). Consider the frame bundle over M^D and a connection σ defining the horizontal lift $\dot{\rho}(t)$ of a vector $\dot{x}(t)$,

$$\dot{\rho}(t) = \sigma(\rho(t)) \cdot \dot{x}(t) \quad [75]$$

In order to bring eqn [75] in the form [64], we think of a frame $u(t)$ as a linear map from \mathbb{R}^D into the tangent space $T_{x(t)}M^D$:

$$u(t): \mathbb{R}^D \rightarrow T_{x(t)}M^D \quad [76]$$

Let

$$\dot{z}(t) := u(t)^{-1} \dot{x}(t) \quad [77]$$

Choose a basis $\{e_{(A)}\}$ in \mathbb{R}^D and $\{e_{(\alpha)}\}$ in $T_{x(t)}M^D$ such that

$$\dot{z}(t) = \dot{z}^A(t) e_{(A)} = u(t)^{-1} (\dot{x}^\alpha(t) e_{(\alpha)}) \quad [78]$$

Insert $u(t) \circ u(t)^{-1}$ into [75], then

$$\dot{\rho}(t) = X_{(A)}(\rho(t)) \dot{z}^A(t) \quad [79]$$

where the dynamical vector fields are

$$X_{(A)}(\rho(t)) = (\sigma(\rho(t)) \circ u(t)) \cdot e_{(A)} \quad [80]$$

The construction [64]–[69] gives a parabolic equation on the bundle. If the connection σ is the metric connection, then the parabolic equation on the bundle gives, by projection on the base space, the parabolic equation with the Laplace–Beltrami operator. Explicitly, the projection on the base space of [67] is

$$\begin{aligned} \psi(t_b, x_b) &:= \int_{\mathcal{P}_b \mathbb{R}^D} \mathcal{D}_{s, Q}(z) \exp\left(-\frac{\pi}{s} Q(z)\right) \\ &\times \phi((\text{Dev } z)(t_a)) \end{aligned} \quad [81]$$

where Dev is the Cartan development map, namely the bijection, defined by [82], from the space of pointed paths z on $T_b M^D$ (identified to \mathbb{R}^D via the

frame u_B) into the space of pointed paths x on M^D (paths such that $x(t_b) = x_b$):

$$(\Pi \circ \rho)(t) =: (\text{Dev } z)(t) \quad [82]$$

Π is the projection on the base space. The path integral [81] is the solution of the equations

$$\frac{\partial}{\partial t_b} \psi(t_b, x_b) = \frac{s}{4\pi} \Delta \psi(t_b, x_b) \quad [83]$$

$$\psi(t_a, x) = \phi(x) \quad [84]$$

where Δ is the Laplace–Beltrami operator on (M^D, g) ,

$$\Delta = g^{ij} D_i D_j \quad [85]$$

and D_i is the covariant derivative defined by the Riemann connection σ .

Semiclassical Expansions

Classical mechanics is a limit of quantum mechanics; therefore, it is natural to expand the action functional S of a given system around, or near, its classical value – namely its minimum $S(q)$, where q is a solution of the Euler–Lagrange equation,

$$S'(q) = 0 \quad [86]$$

Set

$$\begin{aligned} S(x) &= S(q) + S'(q) \cdot \xi + \frac{1}{2!} S''(q) \cdot \xi \xi \\ &+ \frac{1}{3!} S'''(q) \cdot \xi \xi \xi + \dots \end{aligned} \quad [87]$$

where $x \in \mathbb{X}$ is a path

$$x: T \rightarrow M^D$$

and $\xi, \eta \in T_q \mathbb{X}$ is a vector field at $q \in \mathbb{X}$. The second variation of S is called its Hessian

$$S''(q) \xi \eta =: \text{Hess}(q; \xi, \eta) \quad [88]$$

The arena of semiclassical expansions of a functional integral schematically written as

$$I = \int_{\mathbb{X}_{a,b}} \mathcal{D}x \exp(iS(x)/\hbar) \cdot \phi((x(t_a))) \quad [89]$$

consists of the intersection $U_{a,b}$ of two spaces $\mathbb{X}_{a,b} \subset \mathbb{X}$ the space of paths satisfying D initial conditions (a) and D final conditions (b), and $U^{2D}(S)$ the space of critical points of S

$$q \in U^{2D}(S), \quad S'(q) = 0 \quad [90]$$

$$U_{a,b} := \mathbb{X}_{a,b} \cap U^{2D}(S) \quad [91]$$

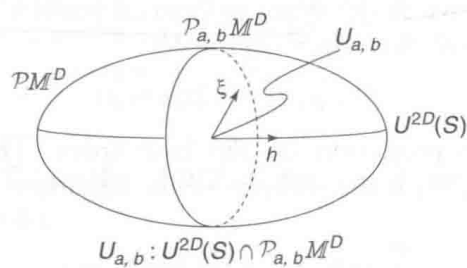


Figure 4 Intersection of the space $\mathcal{P}_{a,b}M^D$ (abbreviated to $\mathbb{X}_{a,b}$) of paths on M^D with fixed points, and the $2D$ -dimensional space $U^{2D}(S)$ of critical points of the system S . (Adapted from a Plenum Press publication with permission by Springer-Verlag.)

The nature of the intersection $U_{a,b}$ determines the behavior of the system S . **Figure 4** shows the intersection of the space $\mathbb{X}_{a,b}$ of paths on M^D with fixed points. It also shows the space $U^{2D}(S)$ of critical points of S .

We consider first the case in which $U_{a,b}$ consists of a single point q , or several isolated points $q_{(i)}$. The semiclassical expansion consists in dropping the terms beyond the Hessian:

$$I_{\text{WKB}} := \int_{\mathbb{X}_b} \mathcal{D}\xi \exp\left(\frac{2\pi i}{h} \left(S(q) + \frac{1}{2} S''(q) \cdot \xi\xi \right)\right) \times \phi(x(t_a)) \tag{92}$$

where the initial wave function ϕ accounts for the D initial conditions of the system, and \mathbb{X}_b is the space of pointed paths

$$x(t_b) = x_b, \text{ and } \xi(t_b) = 0 \quad \text{for every } x \in \mathbb{X}_b \tag{93}$$

WKB Approximations

The integral I_{WKB} is the Gaussian defined by the Hessian. Explicit calculations of I_{WKB} exploit the power of Jacobi fields of S at q .

Example (Momentum-to-position transitions) (e.g., Cartier and DeWitt-Morette 2006). We have

$$I_{\text{WKB}}(x_b, t_b; p_a, t_a) = \exp\frac{2\pi i}{h} S(q(t_b), p(t_a)) \times \left(\det \frac{\partial^2 S}{\partial q^i(t_b) \partial p_j(t_a)} \right)^{1/2} \tag{94}$$

where S is the action function (a.k.a. Hamilton’s principal function)

$$S(q(t_b), p(t_a)) = S(q) + \langle p_a, x(t_a) \rangle \tag{95}$$

where the classical path q is characterized by its initial momentum p_a and its final position x_b . The

proof of [94] rests on the following property of quadratic forms Q . Let $L: X \rightarrow Y$ linearly and

$$Q_X = Q_Y \circ L \tag{96}$$

According to the notations used in [26], [27],

$$\int_X \mathcal{D}_X(x) \exp\left(-\frac{\pi}{s} Q_X(x)\right) = 1 \tag{97}$$

According to [35], [27],

$$1 = \int_X \mathcal{D}_X(x) \exp\left(-\frac{\pi}{s} Q_X(x)\right) = \int_Y \mathcal{D}_Y(Lx) \exp\left(-\frac{\pi}{s} Q_Y(Lx)\right) \tag{98}$$

$$= |\det L| \int \mathcal{D}_Y(x) \exp\left(-\frac{\pi}{s} Q_X(x)\right) \tag{99}$$

If $s = 1$, that is, if Q_X and Q_Y are positive definite, then

$$\int_X \mathcal{D}_Y(x) \exp(-\pi Q_X(x)) = \det(Q_X/Q_Y)^{-1/2} \tag{100}$$

If $s = i$, that is, for Feynman integrals

$$\int_X \mathcal{D}_Y(x) \exp(-\pi Q_X(x)) = |\det(Q_X/Q_Y)|^{-1/2} i^{\text{Ind}(Q_X/Q_Y)} \tag{101}$$

where “ $\text{Ind}(Q_X/Q_Y)$ ” is the ratio of the numbers of negative eigenvalues of Q_X and Q_Y respectively, and $i = \sqrt{-1} = e^{i\pi/2}$.

Equation [100] is a key equation for semiclassical expansions where it is convenient to break up the second variation $S''(q)\xi\xi$ into two quadratic forms:

$$S''(q)\xi\xi = Q_0(\xi) + Q(\xi) \tag{102}$$

where Q_0 is the kinetic energy. The quadratic form Q_0 is a convenient Gaussian volume element for computing [92]. Moreover, splitting the Hessian into $Q_0 + Q$ corresponds to splitting the system into a “free” system and a perturbation.

In eqns [100] and [101] the determinant of the ratios of the infinite-dimensional quadratic forms Q_X/Q_Y have been shown (Cartier and DeWitt-Morette 2006) to be a finite-dimensional determinant, thanks to Jacobi field technology.

Degenerate Hessians; Beyond WKB

When $U_{a,b}$ consists of isolated points, the Hessian is not degenerate, and the semiclassical expansion is usually called the (strict) WKB approximation. When the Hessian is degenerate,

$$S''(q)\xi\xi = 0 \quad \text{for } \xi \neq 0 \tag{103}$$

there is at least one nonzero Jacobi field h along q ,

$$S''(q)h = 0, \quad h \in T_q U^{2D}(S) \quad [104]$$

with D vanishing initial conditions (a) and D vanishing final conditions (b). Equation [104] is the defining equation of Jacobi fields. The vanishing boundary conditions imply that $h \in T_q \mathbb{X}_{a,b}$ as well as being a Jacobi field.

For understanding the intersections $U_{a,b}$ when the Hessian is degenerate, one can construct the following basis for the intersecting tangent spaces $T_q U^{2D}(S)$ and $T_q \mathbb{X}_{a,b}$:

- Basis for $T_q U^{2D}(S)$: a complete set (if it exists) of linearly independent Jacobi fields. It can be constructed by varying the $2D$ conditions (a), (b) satisfied by $q \in \mathbb{X}_{a,b}$.
- Basis for $T_q \mathbb{X}_{a,b}$: a complete set of orthonormal eigenvectors $\{\Psi_k\}$ of the Jacobi operator $\mathcal{J}(q)$ defined by the Hessian

$$S''(q) \cdot \xi \xi =: \langle \langle \mathcal{J}(q), \xi \rangle, \xi \rangle \quad [105]$$

$$\mathcal{J}(q)\Psi_k = \alpha_k \Psi_k, \quad k \in \{0, 1, \dots\} \quad [106]$$

The basis $\{\Psi_k\}$ diagonalizes the Hessian. When the Hessian is degenerate, there is at least one eigenvector of $\mathcal{J}(q)$ with zero eigenvalue.

1. The intersection $U_{a,b}$ is of dimension $l > 0$. Let $\{u^k\}$ be the coordinates of ξ in the $\{\Psi_k\}$ basis of $T_q \mathbb{X}_{a,b}$. Then the diagonalized Hessian is

$$S''(q) \cdot \xi \xi = \sum_{k=0}^{\infty} \alpha_k (u^k)^2 \quad [107]$$

There are l zero eigenvalues $\{\alpha_k\}$ when the system of Euler–Lagrange equations decouples (possibly after a change of variable in $\mathbb{X}_{a,b}$) into two sets: l constraint equations, and $D - l$ equations determining $D - l$ coordinates $\{q^A\}$ of q . Say $l = 1$, for simplicity. Then

$$S(x) = S(q) + c_0 u^0 + \frac{1}{2} \sum_{k=1}^{\infty} \alpha_k (u^k)^2 + \mathcal{O}(|u|^3) \quad [108]$$

where

$$c_0 = \int_T dt \frac{\delta S}{\delta q^j(t)} \Psi_0^j(t) \quad [109]$$

The change of variable $\xi \rightarrow \{u^k\}$ is a linear change of variable of type [33]. The integral [92]

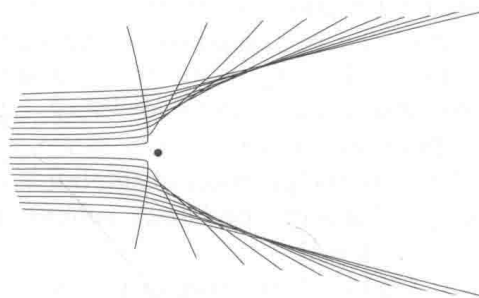


Figure 5 A flow of particles scattered by a repulsive Coulomb potential. (Reprinted from *Physical Review D* with permission by the American Physical Society.)

decomposes into the product of an ordinary integral over u^0 and a Gaussian functional integral defined by a nondegenerate quadratic form. The integral over u^0 yields a Dirac δ -function, $\delta(c_0/h)$. The propagator vanishes unless the conservation law $c_0 = 0$ is satisfied.

Conservation laws appear in the classical limit of quantum physics. The quantum system may have less symmetry than its classical limit.

2. The intersection $U_{a,b}$ is a multiple root of the Euler–Lagrange equation. The flow of classical solutions has an envelope, known as a caustic. Caustics abound in physics: the soap bubble problem, scattering of particles by a repulsive Coulomb potential (see Figure 5), rainbow scattering from a source at infinity, glory scattering etc. (Cartier and DeWitt-Morette 2006).

Let us consider a specific example for simplicity. For instance, the scattering of particles of given momenta p_a by a repulsive Coulomb potential. Let q and q^Δ be two solutions of the Euler–Lagrange equation with slightly different boundary conditions at t_b . Compute $I(x_b^\Delta, t_b; p_a, t_a)$ by expanding the action functional not around q^Δ but around q . The path q^Δ is not in $\mathbb{X}_{a,b}$ and the expansion of the action functional has to be carried up to and including the third variation. As before, let $\{u^k\}$ be the coordinates of ξ in the base $\{\Psi_k\}$, $k \in \{0, 1, \dots\}$. The integral over u^0 is an Airy integral

$$\nu^{-1/3} \text{Ai}(\nu^{-1/3} c) \int_{\mathbb{R}} du^0 \exp\left(i\left(cu^0 + \frac{\nu}{3}(u^0)^3\right)\right) \quad [110]$$

where

$$\nu = \frac{\pi}{\hbar} \int_T dr \int_T ds \int_T dt \frac{\delta^3 S}{\delta q^\alpha(r) \delta q^\beta(s) \delta q^\gamma(t)} \times \Psi_0^\alpha(r) \Psi_0^\beta(s) \Psi_0^\gamma(t) \quad [111]$$

$$c = -\frac{2\pi}{\hbar} \int_T dt \frac{\delta S}{\delta q(t)} \cdot \Psi_0(t) (x_b^\Delta - x_b) \quad [112]$$

The leading contribution of the Airy function when h tends to zero can be computed by the stationary phase method. When x_b^Δ is in the “illuminated” region, the probability amplitude $I(x_b^\Delta, t_b; p_a, t_a)$ oscillates rapidly as h tends to zero. When x_b^Δ is in the “dark” region, the probability amplitude decays exponentially. Quantum mechanics softens up the caustics.

The two kinds of degeneracies described in sections (1) and (2) may occur simultaneously. This happens, for instance, in glory scattering for which the cross section, to leading terms in the semiclassical expansions, has been obtained by functional integration in closed form in terms of Bessel functions (Cartier and DeWitt-Morette 2005).

3. The intersection $U_{a,b}$ is the empty set. There is no classical solution corresponding to the quantum transition. This phenomenon, called “tunneling” or “barrier penetration,” is a rich chapter of quantum physics which can be found in most of the books listed under “Further reading.”

A Multipurpose Tool

Functional integration provides insight and techniques to quantum physics not available from the operator formalism. Just as an example, one can quote the section “Beyond WKB” which has often been dismissed in the operator formalism by stating that “WKB breaks down” in such cases.

The power of functional integration stems from the power of infinite-dimensional spaces. For instance, compare the Lagrangian of a system with its action functional

$$\begin{aligned} S(x) &= \int_T dt L(\dot{x}(t), x(t)), \quad x \in X_{a,b} \\ x: T &\rightarrow M^D, \quad S: X_{a,b} \rightarrow \mathbb{R} \end{aligned} \quad [113]$$

A classical solution q of the system can be defined either by a solution of the Euler–Lagrange equation, together with the boundary conditions dictated by $q \in X_{a,b}$ or by an extremum of the action functional, $S'(q) = 0$. The path q is a significant point in $X_{a,b}$ but it is not isolated and the Hessian $S''(q)$ gives much information on q , such as conservation laws, caustics, tunneling.

A list of applications is beyond the scope of this article. We treat only two applications, then give in the “Further reading” section a short list of books that develop such applications as polarons, phase transitions, properties of quantum gases, scattering processes, many-body theory of bosons and fermions, knot invariants, quantum crystals, quantum field theory, anomalies, etc.

The Homotopy Theorem for Paths Taking Their Values in a Multiply-Connected Space

The space $X_{a,b}$ of paths x

$$x: T \rightarrow M^D, \quad x \in X_{a,b}$$

probes the global properties of their ranges M^D . When M^D is multiply connected, $X_{a,b}$ is the sum of distinct homotopy classes of paths. The integral over $X_{a,b}$ is a linear combination of integrals over each homotopy class of paths. The coefficients of this linear combinations are provided by the homotopy theorem.

The principle of superposition of quantum states requires the probability amplitude for a given transition to be a linear combination of probability amplitudes. It follows that the absolute value of the probability amplitude for a transition from the state a at t_a to the state b at t_b has the form

$$|K(b, t_b; a, t_a)| = \left| \sum_{\alpha} \chi(\alpha) K^{\alpha}(b, t_b; a, t_a) \right| \quad [114]$$

where K^{α} is the interval over paths in the same homotopy class. The homotopy theorem (Laidlaw and Morette-DeWitt 1971) and (Schulman 1971) in Cartier and DeWitt-Morette (2006)) states that the set $\{\chi(\alpha)\}$ forms a representation of the fundamental group of the multiply connected space M^D . One cannot label a homotopy class by an element of the fundamental group unless one has chosen a point $c \in M^D$ and a homotopy class for paths going from c to a and for paths going from c to b – in brief, unless one has chosen a homotopy mesh on M^D . The fundamental group based at c is isomorphic to the fundamental group based at any other point of M^D but not canonically so. Therefore, eqn [114] is only an equality between absolute values of probability amplitudes. The proof of the homotopy theorem consists in requiring [114] to be independent of the chosen homotopy mesh.

Application: Systems of n -Indistinguishable Particles in \mathbb{R}^D

In order that there be a one-to-one correspondence between the system and its configuration space,

$$x: T \rightarrow \mathbb{R}^{D \otimes n} / S_n =: \mathbb{R}^{D,n}$$

where S_n is the symmetric group for n permutations; the coincidence points in $\mathbb{R}^{D,n}$ are excluded so that S_n acts effectively on $\mathbb{R}^{D,n}$. Note that $\mathbb{R}^{1,n}$ is not connected, but $\mathbb{R}^{2,n}$ is multiply connected. When $D \geq 3$, $\mathbb{R}^{D,n}$ is simply connected and the fundamental group on $\mathbb{R}^{D,n}$ is isomorphic to S_n .

There are only two scalar unitary representations of S_n :

$$\begin{aligned} \chi^B : \alpha \in S_n &\rightarrow 1 && \text{for all permutations } \alpha \\ \chi^F : \alpha \in S_n &\rightarrow \begin{cases} 1 & \text{for even permutations} \\ -1 & \text{for odd permutations} \end{cases} \end{aligned}$$

Therefore, in \mathbb{R}^3 there are two different propagators of indistinguishable particles:

$$K^{\text{bose}} = \sum_{\alpha} \chi^B(\alpha) K^{\alpha} \quad [115]$$

is a symmetric propagator

$$K^{\text{fermi}} = \sum_{\alpha} \chi^F(\alpha) K^{\alpha} \quad [116]$$

is an antisymmetric propagator.

The arguments leading to the existence of (scalar) bosons and fermions in \mathbb{R}^3 fails in \mathbb{R}^2 . Statistics cannot be assigned to particles in \mathbb{R}^2 ; particles “without” statistics have been called anyons.

Application: a Spinning Top

Schulman’s analysis of the Schrödinger equation for a spinning top (Schulmann 1968) motivated the formulation of the homotopy theorem. Therefore, Schulman’s results can easily be formulated as an application of [114].

Application: Instantons (DeWitt 2004)

The homotopy theorem reformulated for functional integrals applies to the total $\langle \text{out} | \text{in} \rangle$ amplitude of instantons in Minkowski spacetime.

Scaling Properties of Gaussians

We rewrite the definition [26] of Gaussian volume elements as

$$\int_X d\Gamma_G(x) \exp(-2\pi i \langle x', x \rangle) := \exp(-\pi i W(x')) \quad [117]$$

where the covariance G is defined by the variance W ,

$$W(x') = \langle x', Gx' \rangle$$

In quantum field theory the definition [26] reads

$$\int_{\Phi} d\Gamma_G(\varphi) \exp(-2\pi i \langle J, \varphi \rangle) := \exp(-\pi i W(J)) \quad [118]$$

where φ is a field on spacetime (Minkowski, or Euclidean) and J is called the source. A Gaussian Γ_G can be decomposed into the convolution of any number of Gaussians. For example, if

$$W = W_1 + W_2 \longrightarrow G = G_1 + G_2 \quad [119]$$

then

$$\Gamma_G = \Gamma_{G_1} * \Gamma_{G_2} \quad [120]$$

Explicitly, in QFT

$$\begin{aligned} &\int_{\Phi} d\Gamma_G(\varphi) \exp(-2\pi i \langle J, \varphi \rangle) \\ &= \int_{\Phi} d\Gamma_{G_2}(\varphi_2) \int d\Gamma_{G_1}(\varphi_1) \\ &\quad \times \exp(-2\pi i \langle J, \varphi_1 + \varphi_2 \rangle) \end{aligned} \quad [121]$$

where

$$\varphi = \varphi_1 + \varphi_2 \quad [122]$$

The additive property [119] makes it possible to express a covariance G as an integral over an independent scale variable.

Let $\lambda \in [0, \infty]$ be an independent scale variable. (some authors use $\lambda \in [1, \infty[$ and $\lambda^{-1} \in [0, 1[$). A scale variable has no physical dimension:

$$[\lambda] = 0 \quad [123]$$

The scaling operator S_{λ} acting on a function f of length dimension $[f]$ is by definition

$$S_{\lambda} f(x) := \lambda^{[f]} f(x/\lambda) \quad [124]$$

the scaling of an interval $[a, b[$ is given by $S_{\lambda}[a, b[= \{s/\lambda | s \in [a, b[\}$, that is,

$$S_{\lambda}[a, b[= [a/\lambda, b/\lambda[\quad [125]$$

The scaling of a functional F is

$$(S_{\lambda} F)(\varphi) = F(S_{\lambda} \varphi) \quad [126]$$

In order to decompose a covariance into an integral of scale-dependent contributions we note that a covariance G is a two-point function [31]. In quantum field theory [118], the engineering length dimension of G is twice the field dimension

$$[G] = 2[\varphi] \quad [127]$$

Let $x, y \in \text{spacetime}$ and G be a Laplacian Green function. One can introduce a scaled (truncated) Green function

$$G_{[l_0, l]}(x, y) := \int_{l_0}^l ds S_{s/l_0} u(|x - y|) \quad [128]$$

where

$$\begin{aligned} [l] &= 1, & [s] &= 1, & d^{\times} s &= ds/s \\ l_0 &\leq l, & [u] &= [G] \end{aligned} \quad [129]$$

such that

$$\lim_{l_0=0, l=\infty} G_{[l_0, l]}(x, y) = G(x, y) \quad [130]$$

Example $G(x, y) = c_D/|x - y|^{D-2}$; then the only requirement on the function u in [128] is

$$\int_0^\infty dr r^{-2[\varphi]} u(r) = c_D, \quad [r] = 1 \quad [131]$$

All objects defined by the scaled covariance [128] are labeled with the interval $[l_0, l]$. For instance, a Gaussian volume element $\Gamma_{G[l_0, l]}$ is abbreviated to $\Gamma_{[l_0, l]}$.

A Coarse-Graining Operator

The following coarse-graining operator has been used for constructing a parabolic semigroup equation in the scaling variable (Brydges *et al.* 1998):

$$P_l F := S_{l/l_0} \cdot \Gamma_{[l_0, l]} * F \quad [132]$$

where the convolution product is by definition

$$(\Gamma_{[l_0, l]} * F)(\varphi) = \int_\Phi d\Gamma_{[l_0, l]}(\psi) F(\varphi + \psi)$$

The coarse-graining operator P_l rescales the convolution of a Gaussian volume element $\Gamma_{[l_0, l]}$ so that all volume elements entering the construction of the semigroup renormalization equation are scale independent.

Some properties of the coarse-graining operator:

- $P_{l_2} P_{l_1} = P_{l_2 l_1 / l_0}$.
- The scaled eigenfunctions of the coarse-graining operator are Wick-ordered monomials (Wurm and Berg 2002)

$$P_l : \varphi^n(x) :_{[l_0, \infty]} = \left(\frac{l}{l_0}\right)^{n[\varphi]} : \varphi^n\left(\frac{l_0}{l} x\right) :_{[l_0, \infty]} \quad [133]$$

Note that P_l preserves the scale range.

- Let H be the generator of the coarse-graining operator

$$H := \frac{\partial^\times}{\partial l} P_l \Big|_{l=l_0}, \quad \frac{\partial^\times}{\partial l} = l \frac{\partial}{\partial l} \quad [134]$$

The semigroup renormalization equation (a.k.a. the flow equation)

$$\begin{aligned} \frac{\partial^\times}{\partial l} P_l F(\varphi) &= H P_l F(\varphi) \\ P_{l_0} F(\varphi) &= F(\varphi) \end{aligned} \quad [135]$$

Brydges *et al.* have applied the coarse-graining operator to the quantum field theory known as “ $\lambda\varphi^4$ ” (more precisely the Wick-ordered Lagrangian of $\lambda\varphi^4$). The flow equation [135] plays the role of the “ β -function” equation in perturbative quantum field theory.

Functional Integrals in Quantum Field Theory

Functional integrals in quantum field theory have been modeled to some extent on path integrals in quantum mechanics: mutatis mutandis, the definition [23] of Gaussian volume elements, the diagram expansion [30], the property [36] of linear maps, semiclassical expansions [87], the homotopy theorem [114], and the scaling eqns [135] apply to functional integrals in quantum field theory. The time ordering encoded in a path integral becomes a chronological ordering dictated by light cones in functional integrals of fields on Minkowski fields.

The fundamental difference between quantum mechanics (systems with a finite number of degrees of freedom) and quantum field theory (systems with an infinite number of degrees of freedom) can be said to be “radiative corrections.” In quantum field theory, the concept of “particle” is intrinsically associated to the concept of “field.” A particle is affected by its field. Its mass and charge are modified by the surrounding fields, namely its own and other fields interacting with it. One speaks of “bare mass” and “renormalized mass” when the bare mass is renormalized by surrounding fields. Computing radiative corrections is a delicate procedure because the Green functions G defined by [25] are singular. Regularization techniques have been developed for handling singular Green functions.

Particles in quantum mechanics are simply particles, and bosons and fermions can be treated separately. Not so in quantum field theory. Therefore, the configuration space in quantum field theory is a supermanifold. For functional integrals in this theory, we refer the reader to the “Further reading” section, in particular to the book of A Das for an introduction, to the book of B DeWitt for an in-depth study, and to the book of K Fujikawa and H Suzuki for applications to quantum anomalies.

Concluding Remarks

The key issue in functional integration is the domain of integration, that is, a function space. This infinite-dimensional space, say \mathbb{X} , cannot be considered as the limit $n = \infty$ of \mathbb{R}^n .

Concepts of \mathbb{R}^D stated without reference to D are likely to be meaningful on \mathbb{X} . Other approaches which have been used for exploring \mathbb{X} are

- projective system of finite-dimensional spaces coherently defined on \mathbb{X} (DeWitt-Morette *et al.* 1979),
- one-parameter curves on \mathbb{X} (Figure 1), and
- projecting \mathbb{X} on finite-dimensional spaces (cylindrical integrals).

Functional integration has advanced our understanding of infinite-dimensional spaces, and like all good mathematical tools, it improves with usage.

See also: BRST Quantization; Euclidean Field Theory; Feynman Path Integrals; Infinite-Dimensional Hamiltonian Systems; Knot Theory and Physics; Malliavin Calculus; Path Integrals in Noncommutative Geometry; Quantum Mechanics: Foundations; Stationary Phase Approximation; Topological Sigma Models.

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Γ -Convergence and Homogenization

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Introduction

Several asymptotic problems in the calculus of variations lead to the following question: given a sequence \mathcal{F}_k of functionals, defined on a suitable function space, does there exist a functional \mathcal{F} such that the solutions of the minimum problems for \mathcal{F}_k converge to the solutions of the corresponding minimum problems for \mathcal{F} ? Γ -convergence, introduced by Ennio De Giorgi and his collaborators in 1975, and developed as a powerful tool to attack a wide range of applied problems, provides a unified answer to this kind of question.

Definition and Main Properties

Let \mathcal{U} be a topological space with a countable base and let \mathcal{F}_k be a sequence of functions defined on \mathcal{U} with values in the extended real line $\overline{\mathbf{R}} := \mathbf{R} \cup \{-\infty, +\infty\}$. We say that \mathcal{F}_k Γ -converges to a function $\mathcal{F}: \mathcal{U} \rightarrow \overline{\mathbf{R}}$, or that \mathcal{F} is the Γ -limit of \mathcal{F}_k , if for every $u \in \mathcal{U}$ the following conditions are satisfied:

1. For every sequence u_k converging to u in \mathcal{U} we have

$$\mathcal{F}(u) \leq \liminf_{k \rightarrow \infty} \mathcal{F}_k(u_k)$$

2. There exists a sequence u_k converging to u in \mathcal{U} such that

$$\mathcal{F}(u) = \lim_{k \rightarrow \infty} \mathcal{F}_k(u_k)$$

Property (1) appears to be a variant of the usual definition of lower semicontinuity. Property (2) requires the existence, for every $u \in \mathcal{U}$, of a “recovery sequence,” which provides an approximation of the value of \mathcal{F} at u by means of values attained by \mathcal{F}_k near u .

It follows immediately from the definition that, if \mathcal{F}_k Γ -converges to \mathcal{F} , then $\mathcal{F}_k + \mathcal{G}$ Γ -converges to $\mathcal{F} + \mathcal{G}$ for every continuous function $\mathcal{G}: \mathcal{U} \rightarrow \mathbf{R}$.

The first general property of Γ -limits is lower semicontinuity: if \mathcal{F}_k Γ -converges to \mathcal{F} , then \mathcal{F} is lower semicontinuous on \mathcal{U} ; that is,

$$\mathcal{F}(u) \leq \liminf_{k \rightarrow \infty} \mathcal{F}(u_k)$$

for every $u \in \mathcal{U}$ and for every sequence u_k converging to u in \mathcal{U} .

Another important property of Γ -convergence is compactness: every sequence \mathcal{F}_k has a Γ -convergent subsequence.

For every k assume that the function \mathcal{F}_k has a minimum point u_k . The following property is the link between Γ -convergence and convergence of minimizers: if \mathcal{F}_k Γ -converges to \mathcal{F} and u_k converges to u , then u is a minimum point of \mathcal{F} and $\mathcal{F}_k(u_k)$ converges to $\mathcal{F}(u)$, hence

$$\min_{v \in \mathcal{U}} \mathcal{F}(v) = \lim_{k \rightarrow \infty} \min_{v \in \mathcal{U}} \mathcal{F}_k(v) \quad [1]$$

Under suitable coerciveness assumptions, the convergence of u_k is obtained by a compactness argument. We recall that a sequence of functions \mathcal{F}_k is said to be equicoercive if for every $t \in \mathbf{R}$ there exists a compact set \mathcal{K}_t (independent of k) such that

$$\{u \in \mathcal{U}: \mathcal{F}_k(u) \leq t\} \subset \mathcal{K}_t \quad [2]$$

for every k .

If \mathcal{F}_k is equicoercive and Γ -converges to \mathcal{F} , the previous result implies that [1] holds. If, in addition, \mathcal{F} is not identically $+\infty$, then the sequence u_k of minimizers considered above has a subsequence u_{k_j} which converges to a minimizer u of \mathcal{F} . The whole sequence u_k converges to u whenever \mathcal{F} has a unique minimizer u .

In many applications to the calculus of variations, \mathcal{U} is the Lebesgue space $L^p(\Omega; \mathbf{R}^m)$, with Ω a bounded open subset of \mathbf{R}^n and $1 \leq p < +\infty$, but the effective domains of the functionals \mathcal{F}_k , defined as $\{u \in \mathcal{U}: \mathcal{F}_k(u) \in \mathbf{R}\}$, are often contained in the Sobolev space $W^{1,p}(\Omega; \mathbf{R}^m)$, composed of all functions $u \in L^p(\Omega; \mathbf{R}^m)$ whose distributional gradient

∇u belongs to $L^p(\Omega; \mathbb{R}^{m \times n})$. When one considers homogeneous Dirichlet boundary conditions, the effective domains of the functionals \mathcal{F}_k are often contained in the smaller Sobolev space $W_0^{1,p}(\Omega; \mathbb{R}^m)$, composed of all functions of $W^{1,p}(\Omega; \mathbb{R}^m)$ which vanish on the boundary $\partial\Omega$, technically defined as the closure of $C_0^\infty(\Omega; \mathbb{R}^m)$ in $W^{1,p}(\Omega; \mathbb{R}^m)$.

In this case, the equicoerciveness condition [2] can be obtained by using Rellich's theorem, which asserts that the natural embedding of $W_0^{1,p}(\Omega; \mathbb{R}^m)$ into $L^p(\Omega; \mathbb{R}^m)$ is compact. Therefore, a sequence of functionals \mathcal{F}_k defined on $L^p(\Omega; \mathbb{R}^m)$ is equicoercive if there exists a constant $\alpha > 0$ such that

$$\mathcal{F}_k(u) \geq \alpha \int_{\Omega} |\nabla u|^p dx$$

for every $u \in W_0^{1,p}(\Omega; \mathbb{R}^m)$, while $\mathcal{F}_k(u) = +\infty$ for every $u \notin W_0^{1,p}(\Omega; \mathbb{R}^m)$.

Homogenization Problems

Many problems for composite materials (fibered or stratified materials, porous media, materials with many small holes or fissures, etc.) lead to the study of mathematical models with many interacting scales, which may differ by several orders of magnitude. From a microscopic viewpoint, the systems considered are highly inhomogeneous. Typically, in such composite materials, the physical parameters (such as electric and thermal conductivity, elasticity coefficients, etc.) are discontinuous and oscillate between the different values characterizing each component.

When these components are intimately mixed, these parameters oscillate very rapidly and the microscopic structure becomes more and more complex. On the other hand, the material becomes quite simple from a macroscopic point of view, and it tends to behave like an ideal homogeneous material, called "homogenized material." The purpose of the mathematical theory of homogenization is to describe this limit process when the parameters which describe the fineness of the microscopic structure tend to zero.

Homogenization problems are often treated by studying the partial differential equations that govern the physical properties under investigation. Due to the small scale of the microscopic structure, these equations contain some small parameters. The mathematical problem consists then in the study of the limit of the solutions of these equations when the parameters tend to zero. Γ -convergence is a very useful tool to obtain homogenization results for systems governed by variational principles, which are the only ones described in this article.

Let $Q := (-1/2, 1/2)^n$ be the open unit cube in \mathbb{R}^n centered at 0. We say that a function u defined on \mathbb{R}^n is Q -periodic if, for every $z \in \mathbb{R}^n$ with integer coordinates, we have $u(x+z) = u(x)$ for every $x \in \mathbb{R}^n$.

Let $f: \mathbb{R}^n \times \mathbb{R}^{m \times n} \rightarrow [0, +\infty)$ be a function such that $x \mapsto f(x, \xi)$ is measurable and Q -periodic on \mathbb{R}^n for every $\xi \in \mathbb{R}^{m \times n}$ and $\xi \mapsto f(x, \xi)$ is convex on $\mathbb{R}^{m \times n}$ for every $x \in \mathbb{R}^n$. Given a bounded open set $\Omega \subset \mathbb{R}^n$ and a constant $p > 1$, let $\mathcal{F}_\varepsilon: L^p(\Omega; \mathbb{R}^m) \rightarrow [0, +\infty]$ be the family of functionals defined by

$$\mathcal{F}_\varepsilon(u) := \begin{cases} \int_{\Omega} f(x/\varepsilon, \nabla u) dx & \text{if } u \in W_0^{1,p}(\Omega; \mathbb{R}^m) \\ +\infty & \text{otherwise} \end{cases}$$

In the applications to composite materials, the functional \mathcal{F}_ε represents the energy of the portion of the material occupying the domain Ω . The fact that the energy density depends on x/ε reflects the ε -periodic structure of the material, which implies that the energy density oscillates faster and faster as $\varepsilon \rightarrow 0$.

Assume that there exist two constants $\beta \geq \alpha > 0$ such that

$$\alpha |\xi|^p \leq f(x, \xi) \leq \beta (1 + |\xi|^p) \quad [3]$$

for every $x \in \Omega$ and every $\xi \in \mathbb{R}^{m \times n}$. Then for every sequence $\varepsilon_k \rightarrow 0$ the functionals $\mathcal{F}_{\varepsilon_k}$ Γ -converge to the functional $\mathcal{F}_{\text{hom}}: L^p(\Omega; \mathbb{R}^m) \rightarrow [0, +\infty]$ defined by

$$\mathcal{F}_{\text{hom}}(u) := \begin{cases} \int_{\Omega} f_{\text{hom}}(\nabla u) dx & \text{if } u \in W_0^{1,p}(\Omega; \mathbb{R}^m) \\ +\infty & \text{otherwise} \end{cases} \quad [4]$$

The integrand $f_{\text{hom}}: \mathbb{R}^{m \times n} \rightarrow [0, +\infty)$ is obtained by solving the cell problem

$$f_{\text{hom}}(\xi) := \min_{w \in W_{\text{per}}^{1,p}(Q; \mathbb{R}^m)} \int_Q f(x, \xi + \nabla w) dx \quad [5]$$

where $W_{\text{per}}^{1,p}(Q; \mathbb{R}^m)$ denotes the space of functions $w \in W_{\text{loc}}^{1,p}(\mathbb{R}^n; \mathbb{R}^m)$ which are Q -periodic.

The function f_{hom} is always convex and satisfies [3]. If it is strictly convex, the basic properties of Γ -convergence imply that for every $g \in L^q(\Omega; \mathbb{R}^m)$, with $1/p + 1/q = 1$, the solutions u_ε of the minimum problems

$$\min_{v \in W_0^{1,p}(\Omega; \mathbb{R}^m)} \int_{\Omega} \left[f\left(\frac{x}{\varepsilon}, \nabla v\right) - g(x)v \right] dx \quad [6]$$

converge in $L^p(\Omega; \mathbb{R}^m)$, as $\varepsilon \rightarrow 0$, to the solution u of the minimum problem

$$\min_{v \in W_0^{1,p}(\Omega; \mathbb{R}^m)} \int_{\Omega} [f_{\text{hom}}(\nabla v) - g(x)v] dx \quad [7]$$

Similar results can be proved for nonhomogeneous Dirichlet boundary conditions, as well as for Neumann boundary conditions.

In the special case $m = 1$, $p = 2$, and

$$f(x, \xi) = \frac{1}{2} \sum_{i,j=1}^n a_{ij}(x) \xi_j \xi_i \quad [8]$$

with $a_{ij}(x)$ Q -periodic, the function f_{hom} takes the form

$$f_{\text{hom}}(\xi) = \frac{1}{2} \sum_{i,j=1}^n a_{ij}^{\text{hom}} \xi_j \xi_i$$

for suitable constant coefficients a_{ij}^{hom} .

By considering the Euler equations of the problems [6] and [7] in this special case, from the previous result we obtain the homogenization theorem for symmetric elliptic operators in divergence form, which asserts that for every $g \in L^2(\Omega)$ the solutions u_ε of the Dirichlet problems

$$\begin{aligned} - \sum_{i,j=1}^n D_i \left(a_{ij} \left(\frac{x}{\varepsilon} \right) D_j u_\varepsilon(x) \right) &= g(x) \quad \text{on } \Omega \\ u_\varepsilon(x) &= 0 \quad \text{on } \partial\Omega \end{aligned}$$

converge in $L^2(\Omega)$ to the solution u of the Dirichlet problem

$$\begin{aligned} - \sum_{i,j=1}^n a_{ij}^{\text{hom}} D_i D_j u(x) &= g(x) \quad \text{on } \Omega \\ u(x) &= 0 \quad \text{on } \partial\Omega \end{aligned}$$

An extensive literature is devoted to precise estimates of the homogenized coefficients a_{ij}^{hom} , depending on various structure conditions on the periodic coefficients $a_{ij}(x)$. Some of these estimates are based on a clever use of the variational formula [5].

Explicit formulas for a_{ij}^{hom} are known in the case of layered materials, which correspond to the case where \mathbf{R}^n is periodically partitioned into parallel layers on which the coefficients $a_{ij}(x)$ take constant values.

Easy examples show that, even if the composite material is isotropic at a microscopic layer (i.e., $a_{ij}(x) = a(x)\delta_{ij}$ for some scalar function $a(x)$), the homogenized material can be anisotropic (i.e., $a_{ij}^{\text{hom}} \neq a\delta_{ij}$), due to the anisotropy of the periodic function $a(x)$, which describes the microscopic distribution of the different components of the composite material.

In the vector case $m > 1$, the convexity hypothesis on $\xi \mapsto f(x, \xi)$ is not satisfied by the most interesting functionals related to nonlinear elasticity. If $\xi \mapsto f(x, \xi)$ is not convex, one can still prove that $\mathcal{F}_{\varepsilon_k}$ Γ -converges

to a functional $\mathcal{F}_{\text{hom}} : L^p(\Omega; \mathbf{R}^m) \rightarrow [0, +\infty]$ of the form [4], but this time $f_{\text{hom}} : \mathbf{R}^{m \times n} \rightarrow [0, +\infty)$ cannot be obtained by solving a problem in the unit cell. Instead, it is given by the asymptotic formula

$$f_{\text{hom}}(\xi) := \lim_{R \rightarrow \infty} \frac{1}{R^n} \min_{w \in W_0^{1,p}(Q_R; \mathbf{R}^m)} \int_{Q_R} f(x, \xi + \nabla w) dx$$

where $Q_R := (-R/2, R/2)^n$ is the open cube of side R centered at 0. Similar formulas can be obtained for quasiperiodic integrands f and for stochastic homogenization problems.

In the nonperiodic case one can prove that, if $g_\varepsilon : \mathbf{R}^n \times \mathbf{R}^{m \times n} \rightarrow [0, +\infty)$ are arbitrary Borel functions satisfying [3], with constants independent of ε , and $\mathcal{G}_\varepsilon : L^p(\Omega; \mathbf{R}^m) \rightarrow [0, +\infty]$ are defined by

$$\mathcal{G}_\varepsilon(u) := \begin{cases} \int_\Omega g_\varepsilon(x, \nabla u) dx & \text{if } u \in W_0^{1,p}(\Omega; \mathbf{R}^m) \\ +\infty & \text{otherwise} \end{cases}$$

then there exists a sequence $\varepsilon_k \rightarrow 0$ such that the functionals $\mathcal{G}_{\varepsilon_k}$ Γ -converge to a functional \mathcal{G} of the form

$$\mathcal{G}(u) := \begin{cases} \int_\Omega g(x, \nabla u) dx & \text{if } u \in W_0^{1,p}(\Omega; \mathbf{R}^m) \\ +\infty & \text{otherwise} \end{cases}$$

with g satisfying [3].

In this case, no easy formula provides the integrand $g(x, \xi)$ in terms of simple operations on the integrands $g_{\varepsilon_k}(x, \xi)$. The indirect connection between these integrands can be obtained by introducing the functions $M_\varepsilon(x, \xi, \rho)$ defined, for $x \in \Omega$, $\xi \in \mathbf{R}^{m \times n}$, and $0 < \rho < \text{dist}(x, \partial\Omega)$, by

$$M_\varepsilon(x, \xi, \rho) := \min_{w \in W_0^{1,p}(B(x, \rho))} \int_{B(x, \rho)} g_\varepsilon(y, \xi + \nabla w) dy$$

where $B(x, \rho)$ is the open ball with center x and radius ρ . These functions describe the local behavior of the integrands g_ε in some special minimum problems. The sequence $\mathcal{G}_{\varepsilon_k}$ Γ -converges to \mathcal{G} if and only if

$$\begin{aligned} g(x, \xi) &= \liminf_{\rho \rightarrow 0} \liminf_{k \rightarrow \infty} \frac{M_{\varepsilon_k}(x, \xi, \rho)}{|B(x, \rho)|} \\ &= \limsup_{\rho \rightarrow 0} \limsup_{k \rightarrow \infty} \frac{M_{\varepsilon_k}(x, \xi, \rho)}{|B(x, \rho)|} \end{aligned}$$

for almost every $x \in \Omega$ and every $\xi \in \mathbf{R}^{m \times n}$.

Similar results have also been proved for integral functionals of the form

$$\mathcal{G}_\varepsilon(u) := \begin{cases} \int_\Omega g_\varepsilon(x, u, \nabla u) dx & \text{if } u \in W_0^{1,p}(\Omega; \mathbf{R}^m) \\ +\infty & \text{otherwise} \end{cases}$$

under suitable structure conditions for the integrands g_ε .

Perforated Domains

In some homogenization problems, the integrand is fixed, but the domain depends on a small parameter ε and its boundary becomes more and more fragmented as $\varepsilon \rightarrow 0$. A typical example is given by periodically perforated domains with small holes. Given a bounded open set $\Omega \subset \mathbb{R}^n$ and a compact set $K \subset \mathbb{Q}$, both with smooth boundaries, for every $\varepsilon > 0$ we consider the perforated sets

$$\Omega_\varepsilon := \Omega \setminus \bigcup_{z \in Z_\Omega^\varepsilon} (\varepsilon z + \varepsilon K) \quad [9]$$

where Z_Ω^ε is the set of vectors $z \in \mathbb{R}^n$ with integer coordinates such that $\varepsilon z + \varepsilon \mathbb{Q} \subset \Omega$.

Given $g \in L^2(\Omega)$, let $\mathcal{F}_\varepsilon: L^2(\Omega) \rightarrow [0, +\infty]$ be the functionals defined by

$$\mathcal{F}_\varepsilon(u) := \begin{cases} \int_{\Omega_\varepsilon} \left[\frac{1}{2} |\nabla u|^2 - gu \right] dx & \text{if } u \in W_0^{1,2}(\Omega) \\ +\infty & \text{otherwise} \end{cases} \quad [10]$$

Minimizing [10] is equivalent to solving the mixed problems

$$\begin{aligned} -\Delta u_\varepsilon &= g & \text{on } \Omega_\varepsilon \\ u_\varepsilon &= 0 & \text{on } \partial\Omega \\ \frac{\partial u_\varepsilon}{\partial \nu} &= 0 & \text{on } \partial\Omega_\varepsilon \setminus \partial\Omega \end{aligned} \quad [11]$$

The homogenization formula [5] is still valid, with minor modifications. It leads to a matrix of coefficients a_{ij}^{hom} such that

$$\sum_{i,j=1}^n a_{ij}^{\text{hom}} \xi_j \xi_i := \min_{w \in W_{\text{per}}^{1,2}(\mathbb{Q})} \int_{\mathbb{Q} \setminus K} |\xi + \nabla w|^2 dx$$

for every $\xi \in \mathbb{R}^n$. For every sequence $\varepsilon_k \rightarrow 0$ the Γ -limit of the functionals $\mathcal{F}_{\varepsilon_k}$ is the functional $\mathcal{F}: L^2(\Omega) \rightarrow [0, +\infty]$ defined by

$$\mathcal{F}(u) := \begin{cases} \int_{\Omega} \left[\frac{1}{2} \sum_{i,j=1}^n a_{ij}^{\text{hom}} D_i u D_j u - mgu \right] dx & \text{if } u \in W_0^{1,2}(\Omega) \\ +\infty & \text{otherwise} \end{cases}$$

where $m := |\mathbb{Q} \setminus K|$ is the volume fraction of the sets Ω_ε .

Since a slight modification of the functionals \mathcal{F}_ε satisfies an equicoerciveness condition, it follows from the basic properties of Γ -convergence that the solutions u_ε of the mixed problems [11] in the perforated domains [9], extended to the holes so that u_ε are harmonic on $\Omega \setminus \bar{\Omega}_\varepsilon$ and $u_\varepsilon \in W_0^{1,2}(\Omega)$,

converge in $L^2(\Omega)$ to the solution u of the Dirichlet problem

$$\begin{aligned} - \sum_{i,j=1}^n a_{ij}^{\text{hom}} D_i D_j u &= mg & \text{on } \Omega \\ u &= 0 & \text{on } \partial\Omega \end{aligned}$$

Therefore, the asymptotic effect of the small holes with Neumann boundary condition is a change in the coefficients of the elliptic equation.

In the case of Dirichlet boundary conditions, it is interesting to consider perforated domains with holes of a different size, namely

$$\Omega_\varepsilon := \Omega \setminus \bigcup_{z \in Z_\Omega^\varepsilon} (\varepsilon z + \varepsilon^{n/(n-2)} K) \quad [12]$$

with $\varepsilon^{n/(n-2)}$ replaced by $\exp(-1/\varepsilon^2)$ if $n=2$, while the case $n=1$ gives only trivial results.

Given $g \in L^2(\Omega)$, let $\mathcal{G}_\varepsilon: L^2(\Omega) \rightarrow [0, +\infty]$ be the functionals defined by

$$\mathcal{G}_\varepsilon(u) := \begin{cases} \int_{\Omega_\varepsilon} \left[\frac{1}{2} |\nabla u|^2 - gu \right] dx & \text{if } u \in W_0^{1,2}(\Omega_\varepsilon) \\ +\infty & \text{otherwise} \end{cases} \quad [13]$$

Minimizing [13] is equivalent to solving the Dirichlet problems

$$\begin{cases} -\Delta u_\varepsilon = g & \text{on } \Omega_\varepsilon \\ u_\varepsilon = 0 & \text{on } \partial\Omega_\varepsilon \end{cases} \quad [14]$$

For every sequence $\varepsilon_k \rightarrow 0$ the Γ -limit of the functionals $\mathcal{G}_{\varepsilon_k}$ is the functional $\mathcal{G}: L^2(\Omega) \rightarrow [0, +\infty]$ defined by

$$\mathcal{G}(u) := \begin{cases} \int_{\Omega} \left[\frac{1}{2} |\nabla u|^2 + \frac{\varepsilon}{2} u^2 - gu \right] dx & \text{if } u \in W_0^{1,2}(\Omega) \\ +\infty & \text{otherwise} \end{cases}$$

where, for $n \geq 3$,

$$c := \text{cap}(K) := \inf_{\substack{w \in C_c^\infty(\mathbb{R}^n) \\ w=1 \text{ on } K}} \int_{\mathbb{R}^n} |\nabla w|^2 dx$$

Since a slight modification of the functionals \mathcal{G}_ε satisfies an equicoerciveness condition, it follows from the basic properties of Γ -convergence that the solutions u_ε of the Dirichlet problems [14] in the perforated domains [12], extended as zero on $\Omega \setminus \bar{\Omega}_\varepsilon$, converge in $L^2(\Omega)$ to the solution u of the Dirichlet problem

$$\begin{aligned} -\Delta u + cu &= g & \text{on } \Omega \\ u &= 0 & \text{on } \partial\Omega \end{aligned} \quad [15]$$

In the electrostatic interpretation of these problems, the boundary $\partial\Omega_\varepsilon$ is a conductor kept at potential

zero. The extra term $c u$ in [15] is due to the electric charges induced on $\partial\Omega_\varepsilon$ by the charge distribution g .

These results on Dirichlet and Neumann boundary conditions have been extended to more general functionals and also to a wide class of nonperiodic distributions of small holes.

Dimension Reduction Problems

In the study of thin elastic structures, like plates, membranes, rods, and strings, it is customary to approximate the mechanical behavior of a thin three-dimensional body by an effective theory for two- or one-dimensional elastic bodies. Γ -convergence provides a useful tool for a rigorous deduction of the lower-dimensional theory.

Let us focus on the derivation of plate theory from three-dimensional finite elasticity. The reference configuration of the thin three-dimensional elastic body is a cylinder of the form

$$\Omega_\varepsilon := S \times \left(-\frac{\varepsilon}{2}, \frac{\varepsilon}{2}\right)$$

where $\varepsilon > 0$ and S is a bounded open subset of \mathbf{R}^2 with smooth boundary. We assume that the body is hyperelastic, with stored elastic energy

$$\int_{\Omega_\varepsilon} W(\nabla u) \, dx$$

where $u: \Omega_\varepsilon \rightarrow \mathbf{R}^3$ is the deformation. The energy density $W: \mathbf{R}^{3 \times 3} \rightarrow [0, +\infty]$, depending on the material, is continuous and frame indifferent; that is, $W(QF) = W(F)$ for every rotation Q and every $F \in \mathbf{R}^{3 \times 3}$, where QF denotes the usual product of 3×3 matrices. We assume that W vanishes on the set $SO(3)$ of rotations, is of class C^2 in a neighborhood $SO(3)$, and satisfies the inequality

$$W(F) \geq \alpha \, \text{dist}^2(F, SO(3)) \quad \text{for every } F \in \mathbf{R}^{3 \times 3} \quad [16]$$

with a constant $\alpha > 0$.

Plate theory is obtained in the limit as $\varepsilon \rightarrow 0$ when the densities of the volume forces applied to the body have the form $\varepsilon^2 f(x_1, x_2)$, with $f \in L^2(S; \mathbf{R}^3)$. We assume that f is balanced; that is,

$$\int_{\Omega_\varepsilon} f \, dx = 0, \quad \int_{\Omega_\varepsilon} x \wedge f \, dx = 0$$

Stable equilibria are then obtained by minimizing the functionals

$$\int_{\Omega_\varepsilon} [W(\nabla u) - \varepsilon^2 f \cdot u] \, dx \quad [17]$$

on $W^{1,2}(\Omega_\varepsilon; \mathbf{R}^3)$.

To study the behavior of [17] as $\varepsilon \rightarrow 0$, it is convenient to change variables, so that the scaled deformations $v(x_1, x_2, x_3) := u(x_1, x_2, \varepsilon x_3)$ are defined on the same domain

$$\Omega := S \times \left(-\frac{1}{2}, \frac{1}{2}\right)$$

The scaled energy density $W_\varepsilon: \mathbf{R}^{3 \times 3} \rightarrow [0, +\infty]$ is then defined as

$$W_\varepsilon(F_1|F_2|F_3) := W\left(F_1|F_2|\frac{1}{\varepsilon}F_3\right)$$

where $(F_1|F_2|F_3)$ denotes the 3×3 matrix with columns F_1, F_2 , and F_3 . This implies that

$$\begin{aligned} & \int_{\Omega_\varepsilon} [W(\nabla u) - \varepsilon^2 f \cdot u] \, dx \\ &= \varepsilon \int_{\Omega} [W_\varepsilon(\nabla v) - \varepsilon^2 f \cdot v] \, dx \end{aligned}$$

The asymptotic behavior of the minimizers of these functionals can be obtained from the knowledge of the Γ -limit of the functionals $\mathcal{F}_\varepsilon: L^2(\Omega; \mathbf{R}^3) \rightarrow [0, +\infty]$ defined by

$$\mathcal{F}_\varepsilon(v) := \begin{cases} \frac{1}{\varepsilon^2} \int_{\Omega} W_\varepsilon(\nabla v) \, dx & \text{if } v \in W^{1,2}(\Omega; \mathbf{R}^3) \\ +\infty & \text{otherwise} \end{cases}$$

Let us fix a sequence $\varepsilon_k \rightarrow 0$. The Γ -limit of $\mathcal{F}_{\varepsilon_k}$ turns out to be finite on the set $\Sigma(S; \mathbf{R}^3)$ of all isometric embeddings of S into \mathbf{R}^3 of class $W^{2,2}$; that is, $v \in \Sigma(S; \mathbf{R}^3)$ if and only if $v \in W^{2,2}(S; \mathbf{R}^3)$ and $(\nabla v)^T \nabla v = I$ a.e. on S . The elements of $\Sigma(S; \mathbf{R}^3)$ will be often regarded as maps from Ω into \mathbf{R}^3 , independent of x_3 .

To describe the Γ -limit, we introduce the quadratic form Q_3 defined on $\mathbf{R}^{3 \times 3}$ by

$$Q_3(F) := \frac{1}{2} D^2 W(I)[F, F]$$

which is the density of the linearized energy for the three-dimensional problem, and the quadratic form Q_2 defined on the space of symmetric 2×2 matrices by

$$\begin{aligned} & Q_2 \begin{pmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{pmatrix} \\ &:= \min_{(b_1, b_2, b_3) \in \mathbf{R}^3} Q_3 \begin{pmatrix} a_{11} & a_{12} & b_1 \\ a_{12} & a_{22} & b_2 \\ b_1 & b_2 & b_3 \end{pmatrix} \end{aligned}$$

The Γ -limit of $\mathcal{F}_{\varepsilon_k}$ is the functional $\mathcal{F}: L^2(\Omega; \mathbf{R}^3) \rightarrow [0, +\infty]$ defined by

$$\mathcal{F}(v) := \begin{cases} \frac{1}{12} \int_{\Omega} Q_2(A) \, dx & \text{if } v \in \Sigma(S; \mathbf{R}^3) \\ +\infty & \text{otherwise} \end{cases}$$

where $A(x_1, x_2)$ denotes the second fundamental form of v ; that is,

$$A_{ij} := -D_i D_j v \cdot v \quad [18]$$

with normal vector $\nu := D_1 v \wedge D_2 v$.

The equicoerciveness of the functionals \mathcal{F}_ε in $L^2(\Omega; \mathbb{R}^3)$ is not trivial for this problem: it follows from [16] through a very deep geometric rigidity estimate which generalizes Korn's inequality (see Friesecke *et al.* (2002)). The basic properties of Γ -convergence imply that

$$\begin{aligned} & \min_{u \in W^{1,2}(\Omega_\varepsilon; \mathbb{R}^3)} \int_{\Omega_\varepsilon} [W(\nabla u) - \varepsilon^2 f \cdot u] dx \\ &= \varepsilon^3 \min_{v \in \Sigma(S; \mathbb{R}^3)} \int_S \left[\frac{1}{12} Q_2(A) - f \cdot \nu \right] dx' + o(\varepsilon^3) \end{aligned}$$

with $x' := (x_1, x_2)$ and A defined by [18].

For every $\varepsilon > 0$ let u_ε be a minimizer of [17] and let $v_\varepsilon(x_1, x_2, x_3) := u_\varepsilon(x_1, x_2, \varepsilon x_3)$. Then the basic properties of Γ -convergence imply that there exists a sequence $\varepsilon_k \rightarrow 0$ such that $v_{\varepsilon_k}(x_1, x_2, x_3)$ converges in $L^2(\Omega; \mathbb{R}^3)$ to a solution $v(x_1, x_2)$ of the minimum problem

$$\min_{v \in \Sigma(S; \mathbb{R}^3)} \int_S \left[\frac{1}{12} Q_2(A) - f \cdot \nu \right] dx' \quad [19]$$

These results provide a sound mathematical justification of the reduced two-dimensional theory of plates based on the minimum problem [19].

Similar results have been proved for shells, membranes, rods, and strings.

Phase Transition Problems

The Cahn–Hilliard gradient theory of phase transitions deals with a fluid with mass m , under isothermal conditions, confined in a bounded open subset Ω of \mathbb{R}^n with smooth boundary, whose Gibbs free energy, per unit volume, is a prescribed function W of the density distribution u . Given a small parameter $\varepsilon > 0$, the energy functional $\mathcal{F}_\varepsilon: L^1(\Omega) \rightarrow [0, +\infty]$ has the form

$$\mathcal{F}_\varepsilon(u) := \begin{cases} \int_\Omega [W(u) + \varepsilon^2 |\nabla u|^2] dx & \text{if } u \in A(m) \\ +\infty & \text{otherwise} \end{cases} \quad [20]$$

where $A(m)$ is the set of all functions $u \in W^{1,2}(\Omega)$ with $\int_\Omega u = m$.

We assume that $W: \mathbb{R} \rightarrow [0, +\infty)$ is continuous and that there exist $\alpha, \beta \in \mathbb{R}$, with $\alpha|\Omega| < m < \beta|\Omega|$, such that $W(t) = 0$ if and only if $t = \alpha$ or $t = \beta$. Moreover, we assume that $W(t) \rightarrow +\infty$ as $t \rightarrow \pm\infty$. In the minimization of \mathcal{F}_ε , the Gibbs free energy $W(u)$ favors the functions whose values are close to α

and β , which represent the pure phases, while the gradient term penalizes the transitions between different phases.

It is easy to see that for every sequence $\varepsilon_k \rightarrow 0$ the sequence $\mathcal{F}_{\varepsilon_k}$ Γ -converges to the functional $\mathcal{F}: L^1(\Omega) \rightarrow [0, +\infty]$ defined by

$$\mathcal{F}(u) := \begin{cases} \int_\Omega W(u) dx & \text{if } \int_\Omega u = m \\ +\infty & \text{otherwise} \end{cases}$$

The set $M(\alpha, \beta, m)$ of minimum points of \mathcal{F} is composed of all measurable functions u on Ω which take only the values α and β (on E_α and E_β , respectively), and satisfy the mass constraint $\alpha|E_\alpha| + \beta|E_\beta| = m$, which is equivalent to

$$|E_\alpha| = \frac{\beta|\Omega| - m}{\beta - \alpha} \quad [21]$$

From the basic properties of Γ -convergence, we deduce that

$$\min_{u \in A(m)} \int_\Omega [W(u) + \varepsilon^2 |\nabla u|^2] dx \rightarrow 0 \quad [22]$$

and that there exists a sequence $\varepsilon_k \rightarrow 0$ such that the minimizers u_{ε_k} of $\mathcal{F}_{\varepsilon_k}$ converge in $L^1(\Omega)$ to a function u which takes only the values α and β and satisfies [21].

This result can be improved by considering the rescaled functionals

$$\mathcal{G}_\varepsilon(u) := \frac{1}{\varepsilon} \mathcal{F}_\varepsilon(u) \quad [23]$$

where \mathcal{F}_ε is defined by [20]. Then for every sequence $\varepsilon_k \rightarrow 0$ the sequence $\mathcal{G}_{\varepsilon_k}$ Γ -converges to the functional $\mathcal{G}: L^1(\Omega) \rightarrow [0, +\infty]$ defined by

$$\mathcal{G}(u) := \begin{cases} 2cP(E_\alpha, \Omega) & \text{if } u \in M(\alpha, \beta, m) \\ +\infty & \text{otherwise} \end{cases}$$

where

$$c := \int_\alpha^\beta \sqrt{W(t)} dt$$

and

$$\begin{aligned} & P(E, \Omega) \\ &:= \sup \left\{ \int_E \operatorname{div} \varphi dx : \varphi \in C_c^1(\Omega; \mathbb{R}^n), |\varphi| \leq 1 \right\} \end{aligned}$$

is the Caccioppoli–De Giorgi perimeter of E in Ω , which coincides with the $(n-1)$ -dimensional measure of $\Omega \cap \partial E$ when E is smooth enough.

Note that the effective domain $A(m)$ of the functionals \mathcal{G}_ε is disjoint from the effective domain of the limit functional \mathcal{G} , which is the set of all functions $u \in M(\alpha, \beta, m)$ with $P(E_\alpha, \Omega) < +\infty$.

As the functionals [20] and [23] have the same minimizers, we deduce that there exists a sequence $\varepsilon_k \rightarrow 0$ such that the minimizers u_{ε_k} of $\mathcal{F}_{\varepsilon_k}$ converge in $L^1(\Omega)$ to a function u which takes only the values α and β , satisfies [21], and fulfills the minimal interface criterion

$$P(E_\alpha, \Omega) \leq P(E, \Omega)$$

for every measurable set $E \subset \Omega$ with $|E| = |E_\alpha|$. Moreover, [22] can be improved, and we obtain

$$\min_{u \in W^{1,2}(\Omega)} \mathcal{F}_\varepsilon(u) = \varepsilon 2cP(E_\alpha, \Omega) + o(\varepsilon)$$

Similar results have been proved when the term $|\nabla u|^2$ in [20] is replaced by a general quadratic form like [8], which leads to an anisotropic notion of perimeter.

Free-Discontinuity Problems

Free-discontinuity problems are minimum problems for functionals composed of two terms of different nature: a bulk energy, typically given by a volume integral depending on the gradient of an unknown function u ; and a surface energy, given by an integral on the unknown discontinuity surface of u . These problems arise in many different fields of science and technology, such as liquid crystals, fracture mechanics, and computer vision.

The prototype of free-discontinuity problems is the minimum problem proposed by David Mumford and Jayant Shah:

$$\min_{(u,K) \in \mathcal{A}} \left\{ \int_{\Omega \setminus K} |\nabla u|^2 dx + \mathcal{H}^{n-1}(K \cap \Omega) + \int_{\Omega \setminus K} |u - g|^2 dx \right\} \quad [24]$$

where Ω is a bounded open subset of \mathbb{R}^n , \mathcal{H}^{n-1} denotes the $(n-1)$ -dimensional Hausdorff measure, $g \in L^\infty(\Omega)$, and \mathcal{A} is the set of all pairs (u, K) with K compact, $K \subset \mathbb{R}^n$, and $u \in C^1(\Omega \setminus K)$.

In the applications to image segmentation problems the dimension n is 2 and the function g represents the grey level of an image. Given a solution (u, K) of the minimum problem [24], the set K is interpreted as the set of the relevant boundaries of the objects in the image, while u provides a smoothed version of the image. The first term in [24] has a regularizing effect, the purpose of the second term is to avoid over-segmentation, while the last term, called “fidelity term,” forces u to be close to g . Of course, in the applications these terms are multiplied by different coefficients, whose relative values are very important for image

segmentation problems, since they determine the strength of the effect of each term. However, the mathematical analysis of the problem can be easily reduced to the case where all coefficients are equal to 1.

To solve [24], it is convenient to introduce a weak formulation of the problem based on the space $\text{GSBV}(\Omega)$ of generalized special functions with bounded variation (see Ambrosio *et al.* (2000)). Without entering into details, here it is enough to say that every $u \in \text{GSBV}(\Omega)$ has, at almost every point, an approximate gradient ∇u in the sense of geometric measure theory. This is a measurable map from Ω into \mathbb{R}^n which coincides with the usual gradient in the sense of distributions on every open subset U of Ω such that $u \in W^{1,1}(U)$.

The functional $\mathcal{F}: L^1(\Omega) \rightarrow [0, +\infty]$ used for the weak formulation of [24] is defined by

$$\mathcal{F}(u) := \begin{cases} \int_{\Omega} |\nabla u|^2 dx + \mathcal{H}^{n-1}(J_u) & \text{if } u \in \text{GSBV}(\Omega) \\ +\infty & \text{otherwise} \end{cases} \quad [25]$$

where J_u is the jump set of u , defined in a measure-theoretical way as the set of points $x \in \Omega$ such that

$$\limsup_{\rho \rightarrow 0} \frac{1}{|B(x, \rho)|} \int_{B(x, \rho)} |u(y) - a| dy > 0$$

for every $a \in \mathbb{R}$.

For every $g \in L^\infty(\Omega)$, the functional

$$\mathcal{F}(u) + \int_{\Omega} |u - g|^2 dx$$

is lower semicontinuous and coercive on $L^1(\Omega)$; therefore, the minimum problem

$$\min_{u \in L^1(\Omega)} \left\{ \mathcal{F}(u) + \int_{\Omega} |u - g|^2 dx \right\} \quad [26]$$

has a solution. The connection with the Mumford-Shah problem is given by the following regularity result, proved by Ennio De Giorgi and his collaborators: if u is a solution of [26] and \bar{J}_u is its closure, then $\mathcal{H}^{n-1}(\Omega \cap (\bar{J}_u \setminus J_u)) = 0$, $u \in C^1(\Omega \setminus \bar{J}_u)$, and (u, \bar{J}_u) is a solution of [24].

Since the numerical treatment of [24] and [26] is quite difficult, Γ -convergence has been used to approximate [26] by means of minimum problems for integral functionals, whose minimizers can be obtained by standard numerical techniques.

Let us consider the nonlocal functionals $\mathcal{F}_\varepsilon: L^1(\Omega) \rightarrow [0, +\infty]$ defined by

$$\mathcal{F}_\varepsilon(u) := \begin{cases} \frac{1}{\varepsilon} \int_{\Omega} f(\varepsilon \text{Av}(|\nabla u|^2, x, \varepsilon)) dx & \text{if } u \in W^{1,2}(\Omega) \\ +\infty & \text{otherwise} \end{cases}$$

where

$$\begin{aligned} \text{Av}(|\nabla u|^2, x, \varepsilon) \\ := \frac{1}{|B(x, \varepsilon) \cap \Omega|} \int_{B(x, \varepsilon) \cap \Omega} |\nabla u(y)|^2 dy \end{aligned}$$

and $f: [0, +\infty) \rightarrow [0, +\infty)$ is any increasing continuous function with $f(0) = 0$, $f'(0) = 1$, and $f(t) \rightarrow 1/2$ as $t \rightarrow +\infty$. Then for every sequence $\varepsilon_k \rightarrow 0$ the sequence $\mathcal{F}_{\varepsilon_k}$ Γ -converges to \mathcal{F} .

Given $g \in L^\infty(\Omega)$, for every $\varepsilon > 0$ let u_ε be a solution of the minimum problem

$$\begin{aligned} \min_{u \in W^{1,2}(\Omega)} \left\{ \frac{1}{\varepsilon} \int_{\Omega} f\left(\varepsilon \text{Av}(|\nabla u|^2, x, \varepsilon)\right) dx \right. \\ \left. + \int_{\Omega} |u - g|^2 dx \right\} \end{aligned}$$

From the basic properties of Γ -convergence it follows that there exists a sequence $\varepsilon_k \rightarrow 0$ such that u_{ε_k} converges in $L^1(\Omega)$ to a solution u of [26], so that (u, \bar{J}_u) is a solution of [24].

Other approximations by nonlocal functionals use finite differences instead of averages of gradients.

A different approximation can be obtained by using the local functionals $\mathcal{G}_\varepsilon: (L^1(\Omega))^2 \rightarrow [0, +\infty]$ defined by

$$\mathcal{G}_\varepsilon(u, v) := \begin{cases} \int_{\Omega} \left[g_{\eta_\varepsilon}(v) |\nabla u|^2 + \frac{\varepsilon}{2} |\nabla v|^2 + \frac{1}{2\varepsilon} h(v) \right] dx \\ \text{if } (u, v) \in (W^{1,2}(\Omega))^2 \\ +\infty \quad \text{otherwise} \end{cases}$$

where $g_{\eta_\varepsilon}(t) := \eta_\varepsilon + t^2$, $0 < \eta_\varepsilon \ll \varepsilon$, and $h(t) := (1-t)^2$ for $0 \leq t \leq 1$, while $h(t) := +\infty$ otherwise. Let $\mathcal{G}: (L^1(\Omega))^2 \rightarrow [0, +\infty]$ be the functional defined by

$$\mathcal{G}(u, v) := \begin{cases} \mathcal{F}(u) & \text{if } v = 1 \text{ a.e. on } \Omega \\ +\infty & \text{otherwise} \end{cases}$$

where \mathcal{F} is defined [25]. Then for every sequence $\varepsilon_k \rightarrow 0$ the sequence $\mathcal{G}_{\varepsilon_k}$ Γ -converges to \mathcal{G} .

Given $g \in L^\infty(\Omega)$, for every $\varepsilon > 0$ let $(u_\varepsilon, v_\varepsilon)$ be a solution of the minimum problem

$$\begin{aligned} \min_{(u,v) \in (W^{1,2}(\Omega))^2} \int_{\Omega} \left[g_{\eta_\varepsilon}(v) |\nabla u|^2 + \frac{\varepsilon}{2} |\nabla v|^2 \right. \\ \left. + \frac{1}{2\varepsilon} h(v) + |u - g|^2 \right] dx \end{aligned} \quad [27]$$

From the basic properties of Γ -convergence it follows that there exists a sequence $\varepsilon_k \rightarrow 0$ such that u_{ε_k} converges in $L^1(\Omega)$ to a solution u of [26], so that (u, \bar{J}_u) is a solution of [24].

The approximation of the solutions of [24] based on [27] has been used to construct numerical algorithms for image segmentation.

Free discontinuity problems similar to [24] appear in the mathematical treatment of Griffith's model in fracture mechanics. In this case, u is a vector-valued function, which represents the deformation of an elastic body, the first term in [24] is replaced by a more general integral functional which represents the energy stored in the elastic region $\Omega \setminus K$, while the second term is interpreted as the energy dissipated to produce the crack K . An approximation based on minimum problems similar to [27] has been used to construct numerical algorithms to study the process of crack growth in brittle materials.

An important research line, connected with these problems, has been developed in the last years to derive the macroscopic theories of fracture mechanics from the microscopic theories of interatomic interactions. Using Γ -convergence, some theories expressed in the language of continuum mechanics can be obtained as limits of discrete variational models on lattices, as the distance between neighboring points tends to zero.

See also: Convex Analysis and Duality Methods; Elliptic Differential Equations: Linear Theory; Free Interfaces and Free Discontinuities: Variational Problems; Geometric Measure Theory; Image Processing: Mathematics; Variational Techniques for Ginzburg–Landau Energies; Variational Techniques for Microstructures.

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Gauge Theoretic Invariants of 4-Manifolds

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Introduction

Poincaré duality is fundamental in the study of manifolds. In the case of an orientable closed manifold X , this duality appears as an isomorphism

$$\psi : H^k(X; \mathbb{Z}) \rightarrow H_{n-k}(X; \mathbb{Z})$$

between integral cohomology and homology. The map ψ is defined by cap product with a chosen orientation class. This article focuses on dimension $n=4$, where Poincaré duality induces a bilinear form Q on $H_2(X; \mathbb{Z})$ by use of the Kronecker pairing

$$Q(\xi, \xi') = \langle \psi^{-1}(\xi), \xi' \rangle \in \mathbb{Z}$$

One of the outstanding achievements of modern topology, the classification of simply connected topological 4-manifolds by Freedman (1982), can be phrased in terms of the intersection pairing Q . Indeed, two simply connected differentiable 4-manifolds X and X' are orientation preservingly homeomorphic if and only if the associated pairings Q and Q' are equivalent. Freedman's classification scheme has been extended to also cover a wide range of fundamental groups, resulting in a fair understanding of topological 4-manifolds (Freedman and Quinn 1990).

When it comes to differentiable 4-manifolds, the situation changes drastically. On the one hand, there is an abundance of topological 4-manifolds which do not admit a differentiable structure at all. On the other hand, there also are topological 4-manifolds supporting infinitely many distinct differentiable structures. A classification of differentiable 4-manifolds up to differentiable equivalence seems out of reach of current technology, even in the most simple cases.

The discrepancy between topological and differentiable 4-manifolds was uncovered by gauge-theoretic methods, applying the concepts of instantons and of monopoles. In order to study these, one has to equip a 4-manifold both with a Riemannian metric and some

additional structure: a Hermitian rank-2 bundle in the case of instantons and a spin^c -structure in the case of monopoles. Given such data, instantons and monopoles arise as solutions to partial differential equations the gauge equivalence classes of which form finite-dimensional moduli spaces. As it turns out, these moduli spaces encode significant information about the differentiable structures of the underlying 4-manifolds.

A decoding of such information contained in the instanton moduli and in the monopole moduli is achieved through Donaldson invariants and Seiberg–Witten invariants, respectively. This article outlines these theories from a mathematical point of view.

Instantons and Donaldson Invariants

Let X denote a closed, connected, oriented differentiable Riemannian 4-manifold. We will consider a principal bundle P over X with fiber a compact Lie group G with Lie algebra \mathfrak{g} . Connections on P form an infinite-dimensional affine space $\mathcal{A}(P) = A_0 + \Omega^1(X; \mathfrak{g}_P)$ modeled on the vector space of 1-forms with values in the adjoint bundle

$$\mathfrak{g}_P = P \times_{\text{Ad}(G)} \mathfrak{g}$$

The curvature $F_A \in \Omega^2(X, \mathfrak{g}_P)$ of a connection A is a \mathfrak{g}_P -valued 2-form satisfying the Bianchi identity $D_A F_A = 0$. The group \mathcal{G} of principal bundle automorphisms of P acts in a natural way on the space of connections with quotient space

$$\mathcal{B}(P) = \mathcal{A}(P)/\mathcal{G}$$

The Yang–Mills functional

$$\text{YM} : \mathcal{A}(P) \rightarrow \mathbb{R}_{\geq 0}$$

associates to a connection A the norm square

$$\|F_A\|^2 = - \int_X \text{tr}(F_A \wedge *F_A)$$

of its curvature. Here $*$ denotes the Hodge star operator defined by the metric on X and the orientation. The metric $-\text{tr} : \mathfrak{g} \otimes \mathfrak{g} \rightarrow \mathbb{R}$ is $\text{Ad}(G)$ -invariant and hence YM is invariant under the

action of \mathcal{G} . In particular, the Yang–Mills functional descends to a function on the space $\mathcal{B}(P)$ of a gauge equivalence class of connections.

The Euler–Lagrange equations for the critical points of YM, called Yang–Mills equations, are of the form

$$D_A(*F_A) = 0$$

and can be derived easily from the formula

$$F_{A+a} = F_A + D_A(a) + [a \wedge a]$$

Satisfying the equations

$$D_A(*F_A) = 0 \quad \text{and} \quad D_A(F_A) = 0$$

a Yang–Mills connection is characterized by the fact that it is harmonic with respect to its own Laplacian.

The bundle $\wedge^2 T^*X$ of 2-forms on X decomposes into (± 1) -eigenbundles of the Hodge operator. This orthogonal splitting leads to a decomposition of curvature forms

$$F_A = F_A^+ + F_A^-$$

into self-dual and anti-self-dual components. The differential form $-(1/4\pi^2)\text{tr}(F_A \wedge F_A)$ represents a characteristic class of the principal bundle P . In particular, the integral

$$\begin{aligned} \kappa(P) &= - \int_X \text{tr}(F_A \wedge F_A) \\ &= \|F_A^+\|^2 - \|F_A^-\|^2 \end{aligned}$$

is independent of the connection A . The Yang–Mills functional therefore is bounded

$$\text{YM}(P) \geq |\kappa(P)|$$

and attains this minimum at connections A which satisfy the equation

$$*F_A = \pm F_A$$

Such connections are either self-dual, anti-self-dual or both, that is, flat, depending on whether $\kappa(P)$ is negative, positive, or zero. The moduli space of instantons on P is the subset of minima of the Yang–Mills functional

$$M(P) = \text{YM}^{-1}(|\kappa(P)|) \subset \mathcal{B}(P)$$

The moduli space thus consists of gauge equivalence classes of connections which are either self-dual or anti-self-dual. Donaldson theory indeed considers anti-self-dual connections on principal bundles with structure group $\text{PU}(2) = \text{SO}(3)$.

The Hodge $*$ operator induces a decomposition of the second cohomology

$$H^2(X) = H_+^2(X) \oplus H_-^2(X)$$

into (± 1) -eigenspaces of dimension b^+ and b^- . Unless specified differently, cohomology groups are meant with real coefficients. In order to simplify the exposition, we will assume X to be simply connected. The Donaldson invariants then are defined if b^+ is odd and greater than 1.

A “homology orientation” consists of an orientation of $H_+^2(X)$ and an integral homology class $c \in H_2(X; \mathbb{Z})$. The Donaldson invariant $D_{X,c} = D_c$ is defined after fixing such a homology orientation. It is a linear function

$$D_c : A(X) \rightarrow \mathbb{R}$$

where $A(X)$ is the graded algebra

$$A(X) = \text{Sym}_*(H_0(X) \oplus H_2(X))$$

in which $H_i(X)$ has degree $(1/2)(4-i)$. The significance of D_c is its functoriality

$$D_{X',f(c)}(f(\alpha)) = D_{X,c}(\alpha)$$

under diffeomorphisms $f : X \rightarrow X'$ which preserve both orientation and homology orientation. Switching the orientation of $H_+^2(X; \mathbb{R})$ reverses the sign of D_c . Similarly,

$$D_{c'} = (-1)^{((c-c')/2)^2} D_c$$

if $c - c' \in 2H_2(X, \mathbb{Z}) \subset H_2(X; \mathbb{Z})$.

The construction of this invariant makes use of the following facts:

1. An $\text{SO}(3)$ principal bundle P over X is determined by its first Pontrjagin number $p_1(P)$ and its Stiefel–Whitney class $w_2(P) \in H^2(X; \mathbb{Z}/2)$. As X is simply connected, this Stiefel–Whitney class admits integer lifts. Let c be such a lift and let c^2 be shorthand for the intersection pairing $Q(c, c)$. A pair (p_1, w_2) is realized by a principal bundle provided it satisfies the relation $p_1 \equiv c^2$ modulo 4.

2. If b^+ is nonvanishing, then for generic metrics on X , the moduli space $M(P)$ is a manifold of dimension

$$-2p_1(P) - 3(1 + b^+)$$

This follows from a transversality theorem whose main ingredient in the Sard–Smale theorem. The dimension is computed by use of the Atiyah–Singer index theorem: to an anti-self-dual connection A on P there is an associated elliptic complex

$$\begin{aligned} 0 \rightarrow \Omega^0(X; \mathfrak{g}_P) &\xrightarrow{D_A} \Omega^1(X; \mathfrak{g}_P) \\ &\xrightarrow{D_A^+} \Omega_+^2(X; \mathfrak{g}_P) \rightarrow 0 \end{aligned}$$

where $\Omega^i(X; \mathfrak{g}_P)$ denotes \mathfrak{g}_P -valued i -forms on X . This complex describes the tangential structure of

the moduli space at the equivalence class of A . The space $\Omega^1(X; \mathfrak{g}_P)$ is the tangent space of $\mathcal{A}(P)$ at A , $\Omega^0(X; \mathfrak{g}_P)$ is the tangent space of the group \mathcal{G} at the identity, and D_A is the differential of the orbit map. The differential operator D_A^+ is the linearization of the anti-self-duality map

$$a \mapsto F_{A+a}^+ = D_A^+(a) + [a \wedge a]^+$$

3. The moduli space $M(P)$ can be oriented if it is a manifold. The orientation depends on an orientation of $H_+^2(X)$ and on a $U(2)$ -principal bundle which has P as its $PU(2)$ -quotient bundle. It is determined by an integer lift of $w_2(P)$. The elliptic complex above then can be compared with a corresponding elliptic complex where the differentials are given by a complex Dirac operator. This leads to an almost-complex structure on the tangent space for each point in the moduli space and in particular to an orientation on the moduli space itself.

4. Over the product $M(P) \times X$ there is a universal $PU(2)$ -bundle \bar{P} with first Pontrjagin class $p_1(\bar{P})$. Taking slant product with the class $-(1/4)p_1(\bar{P})$ results in a homomorphism

$$\mu: H_i(X) \rightarrow H^{4-i}(M(P))$$

5. The moduli space $M(P)$ in general is noncompact. There is an Uhlenbeck compactification $\overline{M(P)}$ describing "ideal instantons." Such an ideal instanton consists of an element $(x_1, \dots, x_n) \in \text{Sym}_n(X)$ and an anti-self-dual connection A' on the principal bundle P' on X with $w_2(P') = w_2(P)$ for which the equality

$$p_1(P') - p_1(P) = 4n$$

of Pontrjagin numbers holds. Uhlenbeck's compactness theorem describes what happens if a sequence of anti-self-dual connections has no convergent subsequence: after passing to a subsequence, the sequence converges to an anti-self-dual connection on the restriction of P to $X \setminus \{x_1, \dots, x_n\}$. This limit connection extends to a connection A' on the principal bundle P' . The functions $|F_{A_n}|^2$ on X converge to the measure

$$|F_{A'}|^2 + \sum_{i=1}^n 8\pi^2 \delta_{x_i}$$

The compactification $\overline{M(P)}$ is a stratified space and not usually a manifold. If $w_2(P) \neq 0$, then the singular set of codimension at least 2 and thus the space $\overline{M(X)}$ carries a fundamental class. In the case $w_2(P) = 0$, such a fundamental class in general can only be defined if $-p_1(P) > 4 + 3b^+$. In practice, this problem can be circumvented by blowing up X and considering bundles with $w_2(P) \neq 0$ over the connected sum $X \# \overline{CP^2}$. Note that the complex

projective plane CP^2 as a complex manifold carries a natural orientation. The notation $\overline{CP^2}$ indicates a reversed orientation.

6. The classes $\mu(\alpha) \in H^2(M(P))$ for $\alpha \in H^2(X)$ extend over the compactification. The same holds for the class $\mu(x)$, where $x \in H_0(X; \mathbb{Z})$ is the generator corresponding to the orientation, as long as $w_2(P) \neq 0$. Otherwise, there are certain dimension restrictions. However, the same blow-up trick as mentioned above allows to handle the case $w_2(P) = 0$ as well.

Now fix an element $c \in H_2(X; \mathbb{Z})$ and let

$$M_c = \bigsqcup_{d \geq 0} \overline{M(P_{c,d})}$$

denote the disjoint union of all moduli spaces of anti-self-dual connections on principal $PU(2)$ -bundles $P_{c,d}$ whose second Stiefel-Whitney class is Poincaré-dual to c modulo 2 and whose Pontrjagin number equals $-d - (3/2)(b^+ + 1)$.

Our assumption of b^+ being odd corresponds to the fact that the dimension $2d$ of the moduli space $M(c, d)$ is even and congruent to $-c^2 + (1/2)(1 + b^+)$ modulo 4. Neglecting the difficulties in the case $w_2(P) = 0$ mentioned above, we may use the cup product on $H^*(M_c)$ to extend μ to an algebra homomorphism

$$\mu: A(X) \rightarrow H^*(M_c)$$

The Donaldson invariant D_c is nonzero only on elements z of $A(X)$ whose total degree d is congruent to $-c^2 + (1/2)(1 + b^+)$ modulo 4. For such an element it is defined by

$$D_c(z) = \langle \mu(z), \overline{M(P_{c,d})} \rangle = \int_{\overline{M(P_{c,d})}} \mu(z)$$

The Donaldson series D_c is defined as a formal power series

$$D_c(\alpha) = D_c(\exp(\hat{\alpha})) = \sum_{d=0}^{\infty} \frac{D_c(\hat{\alpha}^d)}{d!}$$

for $\alpha \in H_2(X)$ and $\hat{\alpha} = (1 + (x/2))\alpha$.

Computations and Structure Theorems

The first results about these invariants are due to S. Donaldson. He proved both a vanishing and a nonvanishing theorem (Donaldson and Kronheimer 1990):

Theorem 1 *If both $b^+(X) > 0$ and $b^+(Y) > 0$, then all Donaldson invariants vanish for the connected sum $X \# Y$.*

Theorem 2 If c represents a divisor on a complex algebraic surface X and α represents an ample divisor, then

$$D_c(\alpha^r) \neq 0 \quad \text{for } r \gg 0$$

The second theorem is a consequence of the fact that in the case of an algebraic surface the instanton moduli can be described in algebraic geometric terms: the moduli space $\overline{M}(P_{c,d})$ associated to the metric induced from the Fubini–Study metric on $\mathbb{C}P^n$ by an embedding $X \hookrightarrow \mathbb{C}P^n$ carries the structure of a projective variety. This variety is reduced and of complex dimension d , as soon as d is large enough. Furthermore, $\mu(d)$ is the first Chern class of an ample line bundle.

The translation of instanton moduli into algebraic geometry uses two steps: suppose the first Chern class of a $U(r)$ -principal bundle P on a Kähler surface is also the first Chern class of a holomorphic line bundle. Then the absolute minima of the Yang–Mills functional are achieved by Hermite–Einstein connections. These are connections for which the Ricci curvature is a constant multiple of the identity. The second step, the translation from differential geometry into algebraic geometry, is called the Kobayashi–Hitchin correspondence, which again was proved by Donaldson.

The Donaldson invariants have been computed for a number of 4-manifolds. A simply connected 4-manifold is said to have simple type, if the relation

$$D_c(x^2 z) = 4D_c(z)$$

is satisfied by its Donaldson invariant for all $z \in A(X)$ and $c \in H_2(X; \mathbb{Z})$. It is known that this simple type condition holds for many 4-manifolds. Indeed, it is an open question whether there are 4-manifolds which are not of simple type. For manifolds of simple type the Donaldson series \mathbb{D}_c completely determines the Donaldson invariant D_c . A main result is due to Kronheimer and Mrowka (1995):

Theorem 3 Let X be a simply connected 4-manifold of simple type. Then, there exist finitely many basic classes $\kappa_1, \dots, \kappa_n \in H_2(X; \mathbb{Z})$ such that

$$\mathbb{D}_c = \exp(Q/2) \sum_{i=1}^n (-1)^{(c^2 - \kappa_i c)/2} a_i \exp(\kappa_i) \quad .$$

as analytic functions on $H_2(X)$. The numbers a_i are rational and each basic class κ_i is characteristic, that is, it satisfies $\alpha^2 \equiv Q(\alpha, \kappa_i) \pmod{2}$ for all $\alpha \in H_2(X; \mathbb{Z})$. The homology class κ_i in this formula acts on an arbitrary homology class by intersection.

The geometric significance of the basic classes is underlined by the following theorem (Kronheimer and Mrowka 1995):

Theorem 4 If $\alpha \in H_2(X; \mathbb{Z})$ is represented by an embedded surface of genus g with self-intersection $\alpha^2 \geq 2$, then for each basic class κ the following adjunction inequality is satisfied:

$$2g - 2 \geq \alpha^2 + |Q(\kappa, \alpha)|$$

There are many 4-manifolds for which the Donaldson series have been computed (Friedman and Morgan 1997). The basic classes for complete intersections, for example, are the canonical divisor and its negative. Another example is given by elliptic surfaces. Let $E(n; p, q)$ be a minimal elliptic surface, that is, a holomorphic surface admitting a holomorphic map to $\mathbb{C}P^1$ with generic fiber f an elliptic curve. For any numbers n, p , and q with $p < q$ coprime, there exists such a simply connected elliptic surface with Euler characteristic $12n$ and two multiple fibers of multiplicity p and q , respectively. The Donaldson series of $E(n; p, q)$ for $c = 0$ then is given by

$$\mathbb{D} = \exp\left(\frac{Q}{2}\right) \frac{\sinh^n(f)}{\sinh(f/p) \sinh(f/q)}$$

Another important formula relates the Donaldson series \mathbb{D} a manifold X of simple type and the Donaldson series $\hat{\mathbb{D}}$ of the blow-up $X \# \mathbb{C}P^2$:

$$\hat{\mathbb{D}}_c = \mathbb{D}_c \cdot \exp(-e^2/2) \cosh(e)$$

$$\hat{\mathbb{D}}_{c+e} = -\mathbb{D}_c \cdot \exp(-e^2/2) \sinh(e)$$

Here $e \in H_2(\overline{\mathbb{C}P^2}; \mathbb{Z})$ denotes a generator. Indeed, a more general blow-up formula is known which relates the Donaldson invariants for X and its blow-up even in case X is not of simple type. This formula, due to Fintushel and Stern (1996), involves Weierstraß sigma-functions.

The instanton moduli space carries nontrivial information about 4-manifolds even in the case $b^+(X) \leq 1$. However, one has to deal with singularities in the moduli space. Let us first consider the case $b^+(X) = 0$. If the intersection form on X is negative definite, the instanton moduli spaces in general are bound to have singularities. Indeed, Donaldson examined the case with the Pontrjagin number $p_1(P) = -4$ and $w_2(P) = 0$. In this case, the moduli space for a generic metric on X will be an orientable smooth manifold except at isolated singular points. The singularities are cones over $\overline{\mathbb{C}P^2}$ and they correspond to reducible connections, that is, reductions of the structure group of P to $U(1)$. These reductions are in bijective correspondence to pairs $\pm \alpha \in H_2(X; \mathbb{Z})$ with $\alpha^2 = -1$. The Uhlenbeck compactification of the moduli space thus leads to an oriented cobordism between X and the disjoint union $\sqcup_{\alpha} \overline{\mathbb{C}P^2}$ over all pairs $\pm \alpha$ in $H_2(X; \mathbb{Z})$ of square -1 . As the signature of a

manifold is an invariant of oriented cobordism, there have to be b^- many pairs $\pm\alpha$ of square (-1) in $H_2(X; \mathbb{Z})$ and, in particular, the intersection form Q is represented by the negative of the identity matrix (Donaldson 1983):

Theorem 5 *The intersection form on a differentiable manifold with negative-definite intersection form is diagonal.*

Indeed, from rank 8 on there are lots of definite unimodular forms which are not diagonal. By Freedman's (1982) classification, any unimodular form is realized as the intersection form of a simply connected topological manifold. This theorem shows that most of these manifolds do not support differentiable structures.

The case $b^+(X) = 1$ is also interesting. Here, the moduli space is a smooth manifold for a generic metric, giving rise to Donaldson invariants. However, over a smooth path of metrics, there is in general no smooth cobordism of moduli spaces. So the invariants depend on the chosen metric. The singularities in the cobordisms again correspond to classes in $H_2(X; \mathbb{Z})$ with negative square. An analysis of these singularities leads to wall-crossing formulas describing how different choices of the metric do affect Donaldson invariants. The case of CP^2 is special, as there are no elements of negative square in $H_2(CP^2; \mathbb{Z})$. The Donaldson invariants for CP^2 as well as the wall-crossing formulas turn out to be closely related to modular forms (Göttsche 2000).

Monopoles and Seiberg-Witten Invariants

A spin^c -structure on an oriented Riemannian 4-manifold is a $\text{Spin}^c(4)$ -principal bundle P projecting to the orthonormal tangent frame bundle \bar{P} over X through the group homomorphism $\text{Spin}^c(4) \rightarrow \text{SO}(4)$ with kernel $U(1)$. The group $H^2(X; \mathbb{Z})$ acts freely and transitively on the set of all spin^c -structures. A spin^c -connection is a lift to P of the Levi-Civita connection on \bar{P} . Fixing a background spin^c -connection A_0 , the monopole map

$$\mu : (A, \phi) \mapsto (\mathcal{D}_A \phi, F_A^+ - \phi \phi_o^*, d^* a)$$

is defined (Witten 1994) for spin^c -connections $A \in A_0 + \Omega^1(X; i\mathbb{R})$ and positive spinors ϕ . Here, \mathcal{D}_A denotes the complex Dirac operator associated to A and $d^* a$ for $a \in \Omega^1(X; i\mathbb{R})$ is the adjoint of the de Rham differential on forms. The section $\phi \phi_o^*$ of the traceless endomorphism bundle of positive spinors is viewed as a self-dual 2-form on X .

In case the first Betti number vanishes, this map – after suitable Sobolev completion – becomes a map between Hilbert spaces $\mu : \mathcal{A} \rightarrow \mathcal{C}$ which is a compact deformation of a linear Fredholm map. The Weitzenböck formula can be used to show that preimages under μ of bounded sets in \mathcal{C} are bounded in \mathcal{A} . Furthermore, μ is $U(1)$ -equivariant, where $U(1)$ acts by complex multiplication on spinors and trivially on forms. If $b_1(X) > 0$, the monopole map is a map between Hilbert space bundles over the torus $H^1(X)/H^1(X; \mathbb{Z})$. These properties of the monopole map allow for an interpretation in terms of stable homotopy (Bauer 2004):

Theorem 6 *If the first Betti number of X vanishes, then μ defines an element*

$$[\mu] \in \pi_i^{U(1)}(S^0)$$

in an equivariant stable homotopy group of spheres. The index $i = \text{ind } \mathcal{D}_A - H_+^2(X)$ as an element of the real representation ring $\text{RO}(U(1))$ is determined by the analytic index of the linearization of μ .

In the case $b^+(X) > 1$, these equivariant stable homotopy groups can be identified with nonequivariant stable cohomotopy groups $\pi_{\text{st}}^{b^+-1}(CP^{d-1})$. Here, d denotes the index of the complex Dirac operator $\text{ind } \mathcal{D}_A$. Fixing an orientation of $H_+^2(X)$ results in a Hurewicz homomorphism

$$h : \pi_{\text{st}}^{b^+-1}(CP^{d-1}) \rightarrow H^{b^+-1}(CP^{d-1}; \mathbb{Z})$$

If $b^+(X)$ is odd, the image

$$h([\mu]) = \text{SW}(X)t^{(b^+-1)/2}$$

is an integer multiple of a power of the generator $t \in H^2(CP^{d-1}; \mathbb{Z})$. This integer $\text{SW}(X)$ is known as the Seiberg-Witten invariant (Witten 1994).

This invariant alternatively can be defined by considering the moduli space $M(a) = \mu^{-1}(a)$. Assuming $b^+ > 0$, this is a smooth oriented manifold with a free $U(1)$ -action for generic $a \in \Omega^1(X; i\mathbb{R})$. The Seiberg-Witten invariant is the characteristic number obtainable by these data. In general, the stable homotopy invariant $[\mu]$ encodes global information about the monopole map, which cannot be recovered by only considering the moduli space. In case the spin^c -structure is associated to an almost-complex structure, however, there is a fortunate coincidence: the Hurewicz homomorphism in this case is an isomorphism. So for almost-complex spin^c -structures, the invariants $[\mu]$ and SW carry the same information.

The Seiberg-Witten invariants turn out to be directly computable for Kähler manifolds and to some degree also for symplectic manifolds (Taubes 1994). Indeed,

the following theorem follows from arguments of Witten and of Taubes:

Theorem 7 *Let X be a 4-manifold with $b^+ > 1$ and $b_1 = 0$ which can be equipped with a Kähler or a symplectic structure. If $[\mu]$ is nonvanishing for a spin^c -structure on X , then the spin^c -structure is associated to an almost-complex structure. For the canonical spin^c -structure on X the Seiberg–Witten invariant is ± 1 .*

Seiberg–Witten invariants and Donaldson invariants are closely related: Witten gave physical arguments that an equality of the form

$$D = 2^k \exp(Q/2) \cdot \sum_{\alpha} \text{SW}(\alpha) \exp(\alpha)$$

should hold for the Donaldson series for $c=0$ of a simply connected manifold of simple type. Here, $\alpha \in H^2(X; \mathbb{Z})$ denotes the first Chern class of the complex determinant line bundle. This first Chern class characterizes spin^c -structures in the simply connected case. The number k is related to the signature σ and the Euler characteristic χ of the manifold X by the formula

$$4k = 11\sigma + 7\chi + 2$$

A mathematical proof of this formula is known in special cases (Feehan and Leness 2003).

As is the case for Donaldson invariants, the Seiberg–Witten invariants vanish for connected sums $X \# Y$ if both $b^+(X) > 0$ and $b^+(Y) > 0$ holds. This is not the case for the stable homotopy refinement as follows from the following theorem (Bauer 2004).

Theorem 8 *For a connected sum $X \# Y$ of 4-manifolds the stable equivariant homotopy invariants are related by smash product*

$$[\mu_{X \# Y}] = [\mu_X] \wedge [\mu_Y]$$

As an example application, consider connected sums of elliptic surfaces of the form $E(2n; p, q)$. Now suppose X and X' are each connected sums of at most four copies of such elliptic surfaces. Then X and X' are diffeomorphic if and only if the summands were already diffeomorphic. This contrasts to the fact that the connected sum $E(2n; p, q) \# \mathbb{CP}^2$ is diffeomorphic to a connected sum of $4n - 1$ copies of \mathbb{CP}^2 and $20n - 1$ copies of $\overline{\mathbb{CP}}^2$, independently of p and q .

As a final application, we consider the case of spin manifolds. If the manifold X is spin, then the intersection form Q is even, that is, $Q(\alpha, \alpha) = 0 \pmod{2}$ for $\alpha \in H_2(X, \mathbb{Z})$. According to Rochlin's theorem, the signature of a spin 4-manifold is divisible by 16. The monopole map μ for the spin structure admits additional symmetry. It is $\text{Pin}(2)$ -equivariant. The nonabelian group $\text{Pin}(2)$ appears as the normalizer

of the maximal torus $\text{SU}(2)$. Methods from equivariant K -theory lead to Furuta's (2001) theorem:

Theorem 9 *Let X be a spin 4-manifold. Then*

$$\chi(X) > \frac{5}{4} |\sigma(X)|$$

Manifolds with Boundary

Both Donaldson invariants and Seiberg–Witten invariants to some extent satisfy formal properties which fit into a general conceptual framework known as “topological quantum field theories (TQFTs).” Such a TQFT in $3 + 1$ dimensions is a functor on the cobordism category of oriented 3-manifolds to the category of, say, vector spaces over a ground field: it assigns to an oriented 3-manifold Y a vector space $b(Y)$. To a disjoint union it assigns

$$b(Y_1 \sqcup Y_2) = b(Y_1) \otimes b(Y_2)$$

Reversing orientation corresponds to dualizing

$$b(\overline{Y}) = b(Y)^*$$

Viewing a four-dimensional manifold X with boundary $\partial X = \overline{Y}_1 \sqcup Y_2$ formally as a morphism from Y_1 to Y_2 , this functor associates to X a homomorphism

$$\mathcal{H}(X) : b(Y_1) \rightarrow b(Y_2)$$

that is, an element $\mathcal{H}(X) \in b(\overline{Y}_1 \sqcup Y_2)$. The most important feature is the composition law

$$\mathcal{H}(X_1 \cup_Y X_2) = \mathcal{H}(X_2) \circ \mathcal{H}(X_1)$$

So if a cobordism X from Y_1 to Y_2 can be decomposed as a cobordism X_1 from Y_1 to an intermediate submanifold Y and a cobordism X_2 from Y to Y_2 , then the homomorphism $\mathcal{H}(X)$ can be computed from $\mathcal{H}(X_1)$ and $\mathcal{H}(X_2)$ as their composition.

Donaldson invariants and Seiberg–Witten invariants fit neatly into the framework of a TQFT if one restricts to 3-manifolds which are disjoint unions of homology 3-spheres. In both the instanton and the monopole case, the vector spaces $b(Y)$ are Floer homology groups. The construction of Floer homology carries the Morse theory description of the homology of a finite-dimensional manifold over to an infinite-dimensional setting. In the instanton case, one considers the Chern–Simons function

$$\text{CS}(a) = -\frac{1}{8\pi^2} \int_Y \text{tr} \left(a \wedge da + \frac{2}{3} a \wedge a \wedge a \right)$$

This function is defined on the space of gauge equivalence classes of $\text{SU}(2)$ -connections on Y . Note that for a homology 3-sphere, any $\text{SU}(2)$ or $\text{PU}(2)$

principal bundle over Y is trivial. Choosing a trivialization, a connection becomes identified with a Lie-algebra-valued 1-form a . Critical points for the Chern–Simons functional lead to generators in a chain complex the homology of which then gives the Floer groups. Such critical points correspond to flat connections on Y . The Floer homology groups $HF_*(Y)$ are $\mathbb{Z}/8$ -graded in the $SU(2)$ case and $\mathbb{Z}/4$ -graded in the $SO(3)$ case. If X is a 4-manifold with $b_1(X)=0$ and $b^+(X) > 1$ and such that the boundary ∂X is a disjoint union of homology 3-spheres, then the Donaldson invariants are linear maps

$$D_c : A(X) \longrightarrow HF_*(\partial X)$$

These invariants satisfy a composition law on the subring of $A(X)$ generated by two-dimensional homology classes (Donaldson 2002).

In the monopole case, one considers a Chern–Simons–Dirac functional

$$CSD(a, \psi) = \frac{1}{2} \left(\int_Y \langle \psi, \mathcal{D}_a \psi \rangle d\text{vol} - \int_Y a \wedge da \right)$$

and obtains integer graded Floer homology groups. Details and proofs of the relevant composition laws are announced.

See also: Floer Homology; Four-Manifold Invariants and Physics; Gauge Theory: Mathematical Applications; Instantons: Topological Aspects; Moduli Spaces: An Introduction; Several Complex Variables: Basic Geometric Theory; Topological Quantum Field Theory: Overview.

Gauge Theories from Strings

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Introduction

One of the most exciting properties of string theory, which led ten years ago to the formulation of the M theory as the unique theory unifying all interactions, has been the discovery that type II theories, besides a perturbative spectrum consisting of closed-string excitations, contain also a nonperturbative one consisting of “solitonic” p -dimensional objects called Dp branes. They are characterized by two important properties. They are coupled to closed-string states as the graviton, the dilaton, and the R–R $(p+1)$ -form potential, and are described by a classical solution of the low-energy string effective action. Their dynamics is, on the other hand,

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described by open strings having the endpoints attached to their world volume and therefore satisfying Dirichlet boundary conditions in the directions transverse to their world volume. This is the reason why they are called D (Dirichlet) branes. Since the lightest open-string excitation corresponds to a gauge field, they have a gauge theory living on their world volume. This twofold description of D-branes has opened the way to study both the perturbative and nonperturbative properties of the gauge theory living on their world volume from their dynamics in terms of closed strings. With the addition of the decoupling limit, these two properties have led to the Maldacena (1998) conjecture of the equivalence between the maximally supersymmetric and conformal $\mathcal{N}=4$ super Yang–Mills and type IIB string theory on $AdS_5 \times S^5$.

They have also been successfully applied to less supersymmetric and nonconformal gauge theories

that live on the world volume of fractional and wrapped branes. For general reviews of various approaches see Bertolini *et al.* (2000), Herzog *et al.* (2001), Bertolini (2003), Bigazzi *et al.* (2002), and Di Vecchia and Liccardo (2003). Also in these cases, one has constructed a classical solution of the supergravity equations of motion corresponding to these more sophisticated branes. These equations contain not only the supergravity fields present in the bulk ten-dimensional action but also boundary terms corresponding to the location of the branes. It turns out that in general the classical solution develops a naked singularity of the repulson type at short distances from the branes. This means that at short distances, it does not provide a reliable description of the branes. In the case of $\mathcal{N}=2$ supersymmetry, this can be explicitly seen because of the appearance of an enhançon located at distances slightly higher than the naked singularity (Johnson *et al.* 2000). The enhançon radius corresponds, in supergravity, to the distance where a brane probe becomes tensionless, and, in the gauge theory living on the branes, to the dynamically generated scale Λ_{QCD} . Then, since short distances in supergravity correspond to large distances in the gauge theory, as implied by holography, the presence of the enhançon and of the naked singularity does not allow to get any information on the nonperturbative large-distance behavior of the gauge theory living on the D-branes. Above the radius of the enhançon, instead, the classical solution provides a good description of the branes and therefore it can be used to get information on the perturbative behavior of the gauge theory. This shows that, if we want to use the D-branes for studying the nonperturbative properties of the gauge theory living on their world volume, we must construct a classical solution that has no naked singularity at short distances in supergravity. We will see in a specific example that it will be possible to deform the classical solution, eliminating the naked singularity, and use it to describe nonperturbative properties as the gaugino condensate.

In this article, we review some of the results obtained by using fractional D3 branes of some orbifold and D5 branes wrapped on 2-cycles of some Calabi–Yau manifold. The analysis of the supersymmetric gauge theories living on the world volume of these D-branes will be based on the gauge/gravity relations that relate the gauge coupling constant and the θ -angle to the supergravity fields (see, e.g., reference Di Vecchia *et al.* (2005) for a derivation of them):

$$\frac{4\pi}{g_{\text{YM}}^2} = \frac{1}{g_s(2\pi\sqrt{\alpha'})^2} \int_{C_2} d^2\xi e^{-\phi} \sqrt{\det(G_{AB} + B_{AB})} \quad [1]$$

and

$$\theta_{\text{YM}} = \frac{1}{2\pi\alpha' g_s} \int_{C_2} (C_2 + C_0 B_2) \quad [2]$$

where C_2 is the 2-cycle where the branes are wrapped.

In the next section, we will describe the case of the fractional D3 branes of the orbifold C^2/Z_2 and show that the classical solution corresponding to a system of N D3 and M D7 branes reproduces the perturbative behavior of $\mathcal{N}=2$ super-QCD. Then, we will consider D5 branes wrapped on 2-cycles of a Calabi–Yau manifold described by the Maldacena–Núñez classical solution (Maldacena and Núñez 2001, Chamseddine and Volkov 1997) and show that in this case we are able to reproduce the phenomenon of gaugino condensate and to construct the complete β -function of $\mathcal{N}=1$ super Yang–Mills.

Fractional D3 Branes of the Orbifold C^2/Z_2 and $\mathcal{N}=2$ Super-QCD

In this section, we consider fractional D3 and D7 branes of the noncompact orbifold C^2/Z_2 in order to study the properties of $\mathcal{N}=2$ super-QCD. We group the coordinates of the directions (x^4, \dots, x^9) transverse to the world volume of the D3 brane where the gauge theory lives, into three complex quantities: $z_1 = x^4 + ix^5$, $z_2 = x^6 + ix^7$, $z_3 = x^8 + ix^9$. The nontrivial generator h of Z_2 acts as $z_2 \rightarrow -z_2$, $z_3 \rightarrow -z_3$, leaving z_1 invariant. This orbifold has one fixed point, located at $z_2 = z_3 = 0$ and corresponding to a vanishing 2-cycle. Fractional D3 branes are D5 branes wrapped on the vanishing 2-cycle and therefore are, unlike bulk branes, stuck at the orbifold fixed point. By considering N fractional D3 and M fractional D7 branes of the orbifold C^2/Z_2 , we are able to study $\mathcal{N}=2$ super-QCD with M hypermultiplets. In order to do that, we need to determine the classical solution corresponding to the previous brane configuration. For the case of the orbifold C^2/Z_2 , the complete classical solution is found in Bertolini *et al.* (2002b); see also references therein and Bertolini *et al.* (2000) for a review on fractional branes. In the following, we write it explicitly for a system of N fractional D3 branes with their world volume along the directions x^0, x^1, x^2 , and x^3 and M fractional D7 branes containing the D3 branes in their world volume and having the remaining four world-volume directions along the orbifolded ones. The metric,

the 5-form field strength, the axion, and the dilaton are given by

$$ds^2 = H^{-1/2} \eta_{\alpha\beta} dx^\alpha dx^\beta + H^{1/2} (\delta_{\ell m} dx^\ell dx^m + e^{-\phi} \delta_{ij} dx^i dx^j) \quad [3]$$

$$\tilde{F}_{(5)} = d(H^{-1} dx^0 \wedge \dots \wedge dx^3) + *d(H^{-1} dx^0 \wedge \dots \wedge dx^3) \quad [4]$$

$$\tau \equiv C_0 + ie^{-\phi} = i \left(1 - \frac{Mg_s}{2\pi} \log \frac{z}{\epsilon} \right) \quad [5]$$

$$z \equiv x^4 + ix^5 = ye^{i\theta}$$

where the self-dual field strength $\tilde{F}_{(5)}$ is given in terms of the NS-NS and R-R 2-forms B_2 and C_2 and of the 4-form potential C_4 by $\tilde{F}_{(5)} = dC_4 + C_2 \wedge dB_2$. The warp factor H is a function of the coordinates (x^4, \dots, x^9) and ϵ is an infrared cutoff. We denote by α and β the four directions corresponding to the world volume of the fractional D3 brane, by ℓ and m those along the four orbifolded directions x^6, x^7, x^8 , and x^9 , and by i and j the directions x^4 and x^5 that are transverse to both the D3 and the D7 branes. The twisted fields are instead given by $B_2 = \omega_2 b$, $C_2 = \omega_2 c$ where ω_2 is the volume form of the vanishing 2-cycle and

$$be^{-\phi} = \frac{(2\pi\sqrt{\alpha'})^2}{2} \left[1 + \frac{2N-M}{\pi} g_s \log \frac{y}{\epsilon} \right] \quad [6]$$

$$c + C_0 b = -2\pi\alpha' \theta g_s (2N-M)$$

The expression of H (Kirsch and Vaman 2005) shows that the previous solution has a naked singularity of the repulsion type at short distances. On the other hand, if we use a brane probe approaching from infinity the stack of branes, described by the previous classical solution, it can also be seen that the tension of the probe vanishes at a distance that is larger than that of the naked singularity. The point where the probe brane becomes tensionless is called “enhancement” (Johnson *et al.* 2000) and at this point the classical solution does not describe anymore the stack of fractional branes.

Let us now use the gauge/gravity relations given in the introduction, to determine the coupling constants of the world-volume theory from the supergravity solution. In the case of fractional D3 branes of the orbifold C^2/Z_2 , that is characterized by one single vanishing 2-cycle C_2 , the gauge coupling constant given in eqn [1] reduces to

$$\frac{1}{g_{YM}^2} = \frac{1}{4\pi g_s (2\pi\sqrt{\alpha'})^2} \int_{C_2} e^{-\phi} B_2 \quad [7]$$

By inserting the classical solution in eqns [7] and [2], we get the following expressions for the gauge coupling constant and the θ_{YM} angle (Bertolini *et al.* 2002b):

$$\frac{1}{g_{YM}^2} = \frac{1}{8\pi g_s} + \frac{2N-M}{16\pi^2} \log \frac{y^2}{\epsilon^2} \quad [8]$$

$$\theta_{YM} = -\theta(2N-M)$$

Notice that the gauge coupling constant appearing in the previous equation is the “bare” gauge coupling constant computed at the scale $m \sim y/\alpha'$, while the square of the bare gauge coupling constant computed at the cutoff $\Lambda \sim \epsilon/\alpha'$ is equal to $8\pi g_s$.

In the case of an $\mathcal{N}=2$ supersymmetric gauge theory, the gauge multiplet contains a complex scalar field Ψ that corresponds to the complex coordinate z transverse to both the world volume of the D3 brane and the four orbifolded directions: $\Psi \sim z/2\pi\alpha'$. This is another example of holographic identification between a quantity, Ψ , peculiar of the gauge theory living on the fractional D3 branes and another one, the coordinate z , peculiar of supergravity. It allows one to obtain the gauge theory anomalies from the supergravity background. In fact, since we know how the scale and $U(1)$ transformations act on Ψ , from the previous gauge/gravity relation we can deduce how they act on z , namely

$$\Psi \rightarrow se^{2i\alpha} \Psi \iff z \rightarrow se^{2i\alpha} z \implies y \rightarrow sy$$

$$\theta \rightarrow \theta + 2\alpha \quad [9]$$

Those transformations do not leave invariant the supergravity background in eqn [6] and when we use them in eqns [7] and [2], they generate the anomalies of the gauge theory living on the fractional D3 branes. In fact, by acting with those transformations in eqns [8], we get

$$\frac{1}{g_{YM}^2} \rightarrow \frac{1}{g_{YM}^2} + \frac{2N-M}{8\pi^2} \log s \quad [10]$$

$$\theta_{YM} \rightarrow \theta_{YM} - 2\alpha(2N-M)$$

The first equation generates the β -function of $\mathcal{N}=2$ super-QCD with M hypermultiplets given by

$$\beta(g_{YM}) = -\frac{2N-M}{16\pi^2} g_{YM}^3 \quad [11]$$

while the second one reproduces the chiral $U(1)$ anomaly (Klebanov *et al.* 2002, Bertolini *et al.* 2002a). In particular, if we choose $\alpha = 2\pi/(2(2N-M))$, then θ_{YM} is shifted by a factor 2π . But since θ_{YM} is periodic of 2π , this means that the subgroup $Z_{2(2N-M)}$ is not anomalous in perfect agreement with the gauge theory results.

Wrapped D5 Branes and $\mathcal{N} = 1$ Super Yang-Mills

In this section, we will consider the classical solution corresponding to N D5 branes wrapped on a 2-cycle of a noncompact Calabi-Yau space and we use it to study the properties of the gauge theory living on their world volume that can be shown to be $\mathcal{N} = 1$ super Yang-Mills.

We start by writing the classical solution found in Maldacena and Núñez (2001) and Chamseddine and Volkov (1997). It has a nontrivial metric:

$$ds_{10}^2 = e^\Phi \left[dx_{1,3}^2 + \frac{e^{2b}}{\lambda^2} (d\tilde{\theta}^2 + \sin^2 \tilde{\theta} d\tilde{\varphi}^2) \right] + \frac{e^\Phi}{\lambda^2} \left[d\rho^2 + \sum_{a=1}^3 (\sigma^a - \lambda A^a)^2 \right] \quad [12]$$

a 2-form R-R potential

$$C^{(2)} = \frac{1}{4\lambda^2} \left[(\psi + \psi_0) (\sin \theta' d\theta' \wedge d\phi - \sin \tilde{\theta} d\tilde{\theta} \wedge d\tilde{\varphi}) - \cos \theta' \cos \tilde{\theta} d\phi \wedge d\tilde{\varphi} \right] + \frac{a}{2\lambda^2} [d\tilde{\theta} \wedge \sigma^1 - \sin \tilde{\theta} d\tilde{\varphi} \wedge \sigma^2] \quad [13]$$

and a dilaton

$$e^{2\Phi} = \frac{\sinh 2\rho}{2e^b} \quad [14]$$

where

$$e^{2b} = \rho \coth 2\rho - \frac{\rho^2}{\sinh^2 2\rho} - \frac{1}{4} \\ e^{2k} = e^b \frac{\sinh 2\rho}{2} \\ a = \frac{2\rho}{\sinh 2\rho} \quad [15]$$

and

$$A^1 = -\frac{1}{2\lambda} a(r) d\tilde{\theta} \\ A^2 = \frac{1}{2\lambda} a(r) \sin \tilde{\theta} d\tilde{\varphi} \\ A^3 = -\frac{1}{2\lambda} \cos \tilde{\theta} d\tilde{\varphi} \quad [16]$$

with $\rho \equiv \lambda r$ and $\lambda^{-2} = Ng_s \alpha'$. The left-invariant 1-forms of S^3 are

$$\sigma^1 = \frac{1}{2} [\cos \psi d\theta' + \sin \theta' \sin \psi d\phi] \\ \sigma^2 = -\frac{1}{2} [\sin \psi d\theta' - \sin \theta' \cos \psi d\phi] \\ \sigma^3 = \frac{1}{2} [d\psi + \cos \theta' d\phi] \quad [17]$$

with $0 \leq \theta' \leq \pi$, $0 \leq \phi \leq 2\pi$, and $0 \leq \psi \leq 4\pi$. The variables $\tilde{\theta}$ and $\tilde{\varphi}$ describe a two-dimensional sphere and vary in the range $0 \leq \tilde{\theta} \leq \pi$ and $0 \leq \tilde{\varphi} \leq 2\pi$. Before proceeding, here we want to stress the fact that the presence of the function $a(\rho) \neq 0$ makes the solution regular everywhere. This will allow us to use it later on to describe the nonperturbative gaugino condensate property of $\mathcal{N} = 1$ super Yang-Mills.

We can now use the previous solution for computing the running coupling constant and the θ parameter of $\mathcal{N} = 1$ super Yang-Mills (see Di Vecchia *et al.* (2002), Bertolini and Merlatti (2003), and Mück (2003) reviewed in Bertolini (2003), Di Vecchia and Liccardo (2003), and Imeroni (2003)). In order to do that, we have to fix the cycle on which to perform the integrals in eqns [1] and [2]. It turns out that this 2-cycle is specified by

$$\tilde{\theta} = \theta' \cdot \tilde{\varphi} = -\phi, \quad \psi = 0 \quad [18]$$

keeping ρ fixed. If we now compute the gauge couplings on the previous cycle with $B_2 = C_0 = 0$, we get

$$\frac{4\pi^2}{Ng_{\text{YM}}^2} = \rho \coth 2\rho + \frac{1}{2} a(\rho) \cos \psi \quad [19]$$

and

$$\theta_{\text{YM}} = \frac{1}{2\pi g_s \alpha'} \int_{S^2} C_2 = -N(\psi + a(\rho) \sin \psi + \psi_0) \quad [20]$$

where we have kept $\psi \neq 0$ for reasons that will become clear in a moment. Equation [19] shows that the coupling constant is running as a function of the distance ρ from the branes. In order to obtain the correct running of the gauge theory, we have to find a relation between ρ and the renormalization group scale μ . This can be obtained with the following considerations. If we look at the previous solution, it is easy to see that the metric in eqn [12] is invariant under the following transformations:

$$\psi \rightarrow \psi + 2\pi \quad \text{if } a \neq 0 \\ \psi \rightarrow \psi + 2\epsilon \quad \text{if } a = 0 \quad [21]$$

where ϵ is an arbitrary constant. On the other hand, C_2 is not invariant under the previous transformations, but its flux, that is exactly equal to θ_{YM} in eqn [20], changes by an integer multiple of 2π :

$$\theta_{\text{YM}} = \frac{1}{2\pi \alpha' g_s} \int_{C_2} C_2 \rightarrow \theta_{\text{YM}} + \begin{cases} -2\pi N, & \text{if } a \neq 0 \\ -2N\epsilon, & \text{if } a = 0, \epsilon = \frac{\pi k}{N} \end{cases} \quad [22]$$

But since the physics does not change when $\theta_{\text{YM}} \rightarrow \theta_{\text{YM}} + 2\pi$, one gets that the transformation in eqn [22] is an invariance. Notice that also eqn [19] for

the gauge coupling constant is invariant under the transformation in eqn [21]. The previous considerations show that the classical solution and also the gauge couplings are invariant under the Z_2 transformation if $a \neq 0$, while this symmetry becomes Z_{2N} if a is taken to be zero. As a consequence, since in the ultraviolet $a(\rho)$ is exponentially small, we can neglect it and we have a Z_{2N} symmetry, while in the infrared we cannot neglect $a(\rho)$ anymore and we have only a Z_2 symmetry left. This fits very well with the fact that $\mathcal{N}=1$ super Yang–Mills has a nonzero gaugino condensate $\langle \lambda\lambda \rangle$ that is responsible for the breaking of Z_{2N} into Z_2 . Therefore, it is natural to identify the gaugino condensate precisely with the function $a(\rho) \neq 0$ that makes the classical solution regular also at short distances in supergravity (Di Vecchia *et al.* 2002, Apreda *et al.* 2002):

$$\langle \lambda\lambda \rangle \sim \Lambda^3 = \mu^3 a(\rho) \quad [23]$$

This provides the relation between the renormalization group scale μ and the supergravity spacetime parameter ρ . In the ultraviolet (large ρ) $a(\rho)$ is exponentially suppressed and in eqns [19] and [20] we can neglect it obtaining

$$\frac{4\pi^2}{Ng_{\text{YM}}^2} = \rho \coth 2\rho \quad [24]$$

$$\theta_{\text{YM}} = -N(\psi + \psi_0)$$

The chiral anomaly can be obtained by performing the transformation $\psi \rightarrow \psi + 2\epsilon$ and getting

$$\theta_{\text{YM}} \rightarrow \theta_{\text{YM}} - 2N\epsilon \quad [25]$$

This implies that the Z_{2N} transformations corresponding to $\epsilon = \pi k/N$ are symmetries because they shift θ_{YM} by multiples of 2π .

In general, however, eqns [19] and [20] are only invariant under the Z_2 subgroup of Z_{2N} corresponding to the transformation

$$\psi \rightarrow \psi + 2\pi \quad [26]$$

that changes θ_{YM} in eqn [20] as follows:

$$\theta_{\text{YM}} \rightarrow \theta_{\text{YM}} - 2N\pi \quad [27]$$

leaving invariant the gaugino condensate:

$$\langle \lambda^2 \rangle = \mu^3 \frac{16\pi^2}{3Ng_{\text{YM}}^2} e^{-8\pi^2/Ng_{\text{YM}}^2} e^{i\theta_{\text{YM}}/N} \quad [28]$$

Therefore, the chiral anomaly and the breaking of Z_{2N} to Z_2 are encoded in eqns [19] and [20]. Finally, if we put $\psi=0$ in eqn [19], we get

$$\frac{4\pi^2}{Ng_{\text{YM}}^2} = \rho \coth 2\rho - \frac{1}{2}a(\rho) = \rho \tanh \rho \quad [29]$$

This equation taken together with eqn [23] allows us to determine the running coupling constant as a function of μ . From it, we get (Di Vecchia *et al.* 2002, Di Vecchia and Liccardo 2003) the Novikov–Shifman–Vainshtein–Zacharov (NSVZ) β -function plus nonperturbative corrections due to fractional instantons:

$$\beta(g_{\text{YM}}) = -\frac{3Ng_{\text{YM}}^3}{16\pi^2} \frac{1 + \frac{4\pi^2}{Ng_{\text{YM}}^2} \sinh^{-2} \frac{4\pi^2}{Ng_{\text{YM}}^2}}{1 - \frac{Ng_{\text{YM}}^2}{8\pi^2} + \frac{1}{2} \sinh^{-2} \frac{4\pi^2}{Ng_{\text{YM}}^2}} \quad [30]$$

where in the ultraviolet we have approximated ρ with $4\pi^2/(Ng_{\text{YM}}^2) \coth 4\pi^2/(Ng_{\text{YM}}^2)$.

See also: AdS/CFT Correspondence; Anomalies; BF Theories; Brane Construction of Gauge Theories; Gauge Theory: Mathematical Applications; Noncommutative Geometry from Strings; Nonperturbative and Topological Aspects of Gauge Theory; Perturbation Theory and its Techniques; Seiberg–Witten Theory; Superstring Theories.

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Gauge Theory: Mathematical Applications

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Introduction

This article surveys some developments in pure mathematics which have, to varying degrees, grown out of the ideas of gauge theory in mathematical physics. The realization that the gauge fields of particle physics and the connections of differential geometry are one and the same has had wide-ranging consequences, at different levels. Most directly, it has led mathematicians to work on new kinds of questions, often shedding light later on well-established problems. Less directly, various fundamental ideas and techniques, notably the need to work with the infinite-dimensional gauge symmetry group, have found a place in the general world-view of many mathematicians, influencing developments in other fields. Still less directly, the work in this area – between geometry and mathematical physics – has been a prime example of the interaction between these fields which has been so fruitful since the 1970s.

The body of this article is divided into three sections: roughly corresponding to analysis, geometry, and topology. However, the different topics come together in many different ways: indeed the existence of these links between the topics is one of the most attractive features of the area.

Gauge Transformations

For a review of the usual foundational material on connections, curvature, and related differential geometric constructions, the reader is referred to standard texts. We will, however, briefly recall the notions of gauge transformations and gauge fixing. The simplest case is that of abelian gauge theory – connections on a $U(1)$ -bundle, say over \mathbb{R}^3 . In that case the connection form, representing the connection in a local trivialization, is a pure

imaginary 1-form A , which can also be identified with a vector field A . The curvature of the connection is the 2-form dA . Changing the local trivialization by a $U(1)$ -valued function $g = e^{ix}$ changes the connection form to

$$\tilde{A} = A - dg g^{-1} = A - id\chi$$

The forms A, \tilde{A} are two representations of the same geometric object: just as the same metric can be represented by different expressions in different coordinate systems. One may want to fix this choice of representation, usually by choosing A to satisfy the Coulomb gauge condition $d^*A = 0$ (equivalently $\operatorname{div} A = 0$), supplemented by appropriate boundary conditions. Here we are using the standard Euclidean metric on \mathbb{R}^3 . (Throughout this article we will work with positive-definite metrics, regardless of the fact that – at least at the classical level – the Lorentzian signature may have more obvious bearing on physics.) Arranging this choice of gauge involves solving a linear partial differential equation (PDE) for χ .

The case of a general structure group G is not much different. The connection form A now takes values in the Lie algebra of G and the curvature is given by the expression

$$F = dA + \frac{1}{2}[A, A]$$

The change of bundle trivialization is given by a G -valued function and the resulting change in the connection form is

$$\tilde{A} = gAg^{-1} - dg g^{-1}$$

(Our notation here assumes that G is a matrix group, but this is not important.) Again, we can seek to impose the Coulomb gauge condition $d^*A = 0$, but now we cannot linearize this equation as before.

We can carry the same ideas over to a global problem, working on a G -bundle P over a general

Riemannian manifold M . The space of connections on P is an affine space \mathcal{A} : any two connections differ by a bundle-valued 1-form. Now the gauge group \mathcal{G} of automorphisms of P acts on \mathcal{A} and, again, two connections in the same orbit of this action represent essentially the same geometric object. Thus, in a sense we would really like to work on the quotient space \mathcal{A}/\mathcal{G} . Working locally in the space of connections, near to some A_0 , this is quite straightforward. We represent the nearby connections as $A_0 + a$, where a satisfies the analog of the coulomb condition

$$d_A^* a = 0$$

Under suitable hypotheses, this condition picks out a unique representative of each nearby orbit. However, this gauge-fixing condition need not single out a unique representative if we are far away from A_0 : indeed, the space \mathcal{A}/\mathcal{G} typically has, unlike \mathcal{A} , a complicated topology which means that it is impossible to find any such global gauge-fixing condition. As noted above, this is one of the distinctive features of gauge theory. The gauge group \mathcal{G} is an infinite-dimensional group, but one of a comparatively straightforward kind – much less complicated than the diffeomorphism groups relevant in Riemannian geometry for example. One could argue that one of the most important influences of gauge theory has been to accustom mathematicians to working with infinite-dimensional symmetry groups in a comparatively simple setting.

Analysis and Variational Methods

The Yang–Mills Functional

A primary object brought to mathematicians attention by physics is the Yang–Mills functional

$$\text{YM}(A) = \int_M |F_A|^2 d\mu$$

Clearly, $\text{YM}(A)$ is non-negative and vanishes if and only if the connection is flat: it is broadly analogous to functionals such as the area functional in minimal submanifold theory, or the energy functional for maps. As such, one can fit into a general framework associated with such functionals. The Euler–Lagrange equations are the Yang–Mills equations

$$d_A^* F_A = 0$$

For any solution (a Yang–Mills connection), there is a “Jacobi operator” H_A such that the second variation is given by

$$\text{YM}(A + ta) = \text{YM}(A) + t^2 \langle H_A a, a \rangle + O(t^3)$$

The omnipresent phenomenon of gauge invariance means that Yang–Mills connections are never isolated, since we can always generate an infinite-dimensional family by gauge transformations. Thus, as explained in the last section, one imposes the gauge-fixing condition $d_A^* a = 0$. Then the operator H_A can be written as

$$H_A a = \Delta_A a + [F_A, a]$$

where Δ_A is the bundle-valued “Hodge Laplacian” $d_A d_A^* + d_A^* d_A$ and the expression $[F_A, a]$ combines the bracket in the Lie algebra with the action of Λ^2 on Λ^1 . This is a self-adjoint elliptic operator and, if M is compact, the span of the negative eigenspaces is finite dimensional, the dimension being defined to be the index of the Yang–Mills connection A .

In this general setting, a natural aspiration is to construct a “Morse theory” for the functional. Such a theory should relate the topology of the ambient space to the critical points and their indices. In the simplest case, one could hope to show that for any bundle P there is a Yang–Mills connection with index 0, giving a minimum of the functional. More generally, the relevant ambient space here is the quotient \mathcal{A}/\mathcal{G} and one might hope that the rich topology of this is reflected in the solutions to the Yang–Mills equations.

Uhlenbeck’s Theorem

The essential foundation needed to underpin such a “direct method” in the calculus of variations is an appropriate compactness theorem. Here the dimension of the base manifold M enters in a crucial way. Very roughly, when a connection is represented locally in a Coulomb gauge, the Yang–Mills action combines the L^2 -norm of the derivative of the connection form A with the L^2 -norm of the quadratic term $[A, A]$. The latter can be estimated by the L^4 -norm of A . If $\dim M \leq 4$, then the Sobolev inequalities allow the L^4 -norm of A to be controlled by the L^2 -norm of its derivative, but this is definitely not true in higher dimensions. Thus, $\dim M = 4$ is the “critical dimension” for this variational problem. This is related to the fact that the Yang–Mills equations (and Yang–Mills functional) are conformally invariant in four dimensions. For any nontrivial Yang–Mills connection over the 4-sphere, one generates a one-parameter family of Yang–Mills connections, on which the functional takes the same value, by applying conformal transformations corresponding to dilations of \mathbf{R}^4 . In such a family of connections the integrand $|F_A|^2$ – the “curvature density” – converges to a δ -function

at the origin. More generally, one can encounter sequences of connections over 4-manifolds for which YM is bounded but which do not converge, the Yang–Mills density converging to δ -functions. There is a detailed analogy with the theory of the harmonic maps energy functional, where the relevant critical dimension (for the domain of the map) is 2.

The result of Uhlenbeck (1982), which makes these ideas precise, considers connections over a ball $B^n \subset \mathbb{R}^n$. If the exponent $p \geq 2n$, then there are positive constants $\epsilon(p, n), C(p, n) > 0$ such that any connection with $\|F\|_{L^p(B^n)} \leq \epsilon$ can be represented in Coulomb gauge over the ball, by a connection form which satisfies the condition $d^*A = 0$, together with certain boundary conditions, and

$$\|A\|_{L^p_1} \leq C\|F\|_{L^p}$$

In this Coulomb gauge, the Yang–Mills equations are elliptic and it follows readily that, in this setting, if the connection A is Yang–Mills one can obtain estimates on all derivatives of A .

Instantons in Four Dimensions

This result of Uhlenbeck gives the analytical basis for the direct method of the calculus of variations for the Yang–Mills functional over base manifolds M of dimension ≤ 3 . For example, any bundle over such a manifold must admit a Yang–Mills connection, minimizing the functional. Such a statement is definitely false in dimensions ≥ 5 . For example, an early result of Bourguignon and Lawson (1981) and Simons asserts that there is no minimizing connection on any bundle over S^n for $n \geq 5$. The proof exploits the action of the conformal transformations of the sphere. In the critical dimension 4, the situation is much more complicated. In four dimensions, there are the renowned “instanton” solutions of the Yang–Mills equation. Recall that if M is an oriented 4-manifold the Hodge $*$ -operation is an involution of $\Lambda^2 T^*M$ which decomposes the two forms into self-dual and anti-self-dual parts, $\Lambda^2 T^*M = \Lambda^+ \oplus \Lambda^-$. The curvature of a connection can then be written as

$$F_A = F_A^+ + F_A^-$$

and a connection is a self-dual (respectively anti-self-dual) instanton if F_A^- (respectively F_A^+) is 0. The Yang–Mills functional is

$$\text{YM}(A) = \|F_A^+\|^2 + \|F_A^-\|^2$$

while the difference $\|F_A^+\|^2 - \|F_A^-\|^2$ is a topological invariant $\kappa(P)$ of the bundle P , obtained by evaluating a four-dimensional characteristic class

on $[M]$. Depending on the sign of $\kappa(P)$, the self-dual or anti-self-dual connections (if any exist) minimize the Yang–Mills functional among all connections on P . These instanton solutions of the Yang–Mills equations are analogous to the holomorphic maps from a Riemann surface to a Kähler manifold, which minimize the harmonic maps energy functional in their homotopy class.

Moduli Spaces

The instanton solutions typically occur in “moduli spaces.” To fix ideas, let us consider bundles with structure group $\text{SU}(2)$, in which case $\kappa(P) = -8\pi^2 c_2(P)$. For each $k > 0$, we have a moduli space \mathcal{M}_k of anti-self-dual instantons on a bundle $P_k \rightarrow M^4$, with $c_2(P_k) = k$. It is a manifold of dimension $8k - 3$. The general goal of the calculus of variations in this setting is to relate three things:

1. the topology of the space \mathcal{A}/\mathcal{G} of equivalence classes of connections on P_k ;
2. the topology of the moduli space \mathcal{M}_k of instantons; and
3. the existence and indices of other, nonminimal, solutions to the Yang–Mills equations on P_k .

In this direction, a very influential conjecture was made by Atiyah and Jones (1978). They considered the case when $M = S^4$ and, to avoid certain technicalities, work with spaces of “framed” connections, dividing by the restricted group \mathcal{G}_0 of gauge transformations equal to the identity at infinity. Then, for any k , the quotient $\mathcal{A}/\mathcal{G}_0$ is homotopy equivalent to the third loop space $\Omega^3 S^3$ of based maps from the 3-sphere to itself. The corresponding “framed” moduli space $\tilde{\mathcal{M}}_k$ is a manifold of dimension $8k$ (a bundle over \mathcal{M}_k with fiber $\text{SO}(3)$). Atiyah and Jones conjectured that the inclusion $\tilde{\mathcal{M}}_k \rightarrow \mathcal{A}/\mathcal{G}_0$ induces an isomorphism of homotopy groups π_l in a range of dimensions $l \leq l(k)$, where $l(k)$ increases with k . This would be consistent with what one might hope to prove by the calculus of variations if there were no other Yang–Mills solutions, or if the indices of such solutions increased with k .

The first result along these lines was due to Bourguignon and Lawson (1981), who showed that the instanton solutions are the only local minima of the Yang–Mills functional over the 4-sphere. Subsequently, Taubes (1983) showed that the index of a non-instanton Yang–Mills connection P_k is at least $k + 1$. Taubes’ proof used ideas related to the action of the quaternions and the hyper-Kähler structure on the $\tilde{\mathcal{M}}_k$ (see the section on hyper-Kähler quotients). Contrary to some expectations, it was shown by

Sibner *et al.* (1989) that nonminimal solutions do exist; some later constructions were very explicit (Sadun and Segert 1992). Taubes' index bound gave ground for hope that an analytical proof of the Atiyah–Jones conjecture might be possible, but this is not at all straightforward. The problem is that in the critical dimension 4 a mini–max sequence for the Yang–Mills functional in a given homotopy class may diverge, with curvature densities converging to sums of δ -functions as outlined above. This is related to the fact that the \tilde{M}_k are not compact. In a series of papers culminating in a framework for Morse theory for Yang–Mills functional, Taubes (1998) succeeded in proving a partial version of the Atiyah–Jones conjecture, together with similar results for general base manifolds M^4 . Taubes showed that, if the homotopy groups of the moduli spaces stabilize as $k \rightarrow \infty$, then the limit must be that predicted by Atiyah and Jones. Related analytical techniques were developed for other variational problems at the critical dimension involving “critical points at infinity.” The full Atiyah–Jones conjecture was established by Boyer *et al.* but using geometrical techniques: the “explicit” description of the moduli spaces obtained from the Atiyah–Drinfeld–Hitchin–Manin (ADHM) construction (see below). A different geometrical proof was given by Kirwan (1994), together with generalizations to other gauge groups.

There was a parallel story for the solutions of the Bogomolony equation over \mathbb{R}^3 , which we will not recount in detail. Here the base dimension is below the critical case but the analytical difficulty arises from the noncompactness of \mathbb{R}^3 . Taubes succeeded in overcoming this difficulty and obtained relations between the topology of the moduli space, the appropriate configuration space and the higher critical points. Again, these higher critical points exist but their index grows with the numerical parameter corresponding to k . At about the same time, Donaldson (1984) showed that the moduli spaces could be identified with spaces of rational maps (subsequently extended to other gauge groups). The analog of the Atiyah–Jones conjecture is a result on the topology of spaces of rational maps proved earlier by Segal, which had been one of the motivations for Atiyah and Jones.

Higher Dimensions

While the scope for variational methods in Yang–Mills theory in higher dimensions is very limited, there are useful analytical results about solutions of the Yang–Mills equations. An important monotonicity result was obtained by Price (1983). For simplicity, consider a Yang–Mills connection over

the unit ball $B^n \subset \mathbb{R}^n$. Then Price showed that the normalized energy

$$E(A, B(r)) = \frac{1}{r^{n-4}} \int_{|x| \leq r} |F|^2 d\mu$$

decreases with r . Nakajima (1988) and Uhlenbeck used this monotonicity to show that for each n there is an ϵ such that if A is a Yang–Mills connection over a ball with $E(A, B(r)) \leq \epsilon$ then all derivatives of A , in a suitable gauge, can be controlled by $E(A, B(r))$. Tian (2000) showed that if A_i is a sequence of Yang–Mills connections over a compact manifold M with bounded Yang–Mills functional, then there is a subsequence which converges away from a set Z of Hausdorff codimension at least 4 (extending the case of points in a 4-manifold). Moreover, the singular set Z is a minimal subvariety, in a suitably generalized sense.

In higher dimensions, important examples of Yang–Mills connections arise within the framework of “calibrated geometry.” Here, we consider a Riemannian n -manifold M with a covariant constant calibrating form $\Omega \in \Omega_M^{n-4}$. There is then an analog of the instanton equation

$$F_A = \pm * (\Omega \wedge F_A)$$

whose solutions minimize the Yang–Mills functional. This includes the Hermitian Yang–Mills equation over a Kähler manifold (see the section on moment maps) and also certain equations over manifolds with special holonomy groups (Donaldson and Thomas 1998). For these “higher-dimensional instantons,” Tian shows that the singular sets Z that arise are calibrated varieties.

Gluing Techniques

Another set of ideas from PDEs and analysis which has had great impact in gauge theory involves the construction of solutions to appropriate equations by the following general scheme:

1. constructing an “approximate solution,” formed from some standard models using cutoff functions;
2. showing that the approximate solution can be deformed to a true solution by means of an implicit function theorem.

The heart of the second step usually consists of estimates for the relevant linear differential operator. Of course, the success of this strategy depends on the particular features of the problem. This approach, due largely to Taubes, has been particularly effective in finding solutions to the first-order instanton equations and their relatives. (The applicability of the approach is connected to the fact that

such solutions typically occur in moduli spaces and one can often “see” local coordinates in the moduli space by varying the parameters in the approximate solution.) Taubes applied this approach to the Bogomolny monopole equation over \mathbb{R}^3 (Jaffe and Taubes 1980) and to construct instantons over general 4-manifolds (Taubes 1982). In the latter case, the approximate solutions are obtained by transplanting standard solutions over \mathbb{R}^4 – with curvature density concentrated in a small ball – to small balls on the 4-manifold, glued to the trivial flat connection over the remainder of the manifold. These types of techniques have now become a fairly standard part of the armory of many differential geometers, working both within gauge theory and other fields. An example of a problem where similar ideas have been used is Joyce’s construction of constant of manifolds with exceptional holonomy groups (Joyce 1996). (Of course, it is likely that similar techniques have been developed over the years in many other areas, but Taubes’ work in gauge theory has done a great deal to bring them into prominence.)

Geometry: Integrability and Moduli Spaces

The Ward Correspondence

Suppose that S is a complex surface and ω is the 2-form corresponding to a Hermitian metric on S . Then S is an oriented Riemannian 4-manifold and ω is a self-dual form. The orthogonal complement of ω in Λ^+ can be identified with the real parts of forms of type $(0,2)$. Hence, if A is an anti-self-dual instanton connection on a principle $U(r)$ -bundle over S the $(0,2)$ part of the curvature of A vanishes. This is the integrability condition for the $\bar{\partial}$ -operator defined by the connection, acting on sections of the associated vector bundle $E \rightarrow S$. Thus, in the presence of the connection, the bundle E is naturally a holomorphic bundle over S .

The Ward correspondence (Ward 1877) builds on this idea to give a complete translation of the instanton equations over certain Riemannian 4-manifolds into holomorphic geometry. In the simplest case, let A be an instanton on a bundle over \mathbb{R}^4 . Then, for any choice of a linear complex structure on \mathbb{R}^4 , compatible with the metric, A defines a holomorphic structure. The choices of such a complex structure are parametrized by a 2-sphere; in fact, the unit sphere in $\Lambda^+(\mathbb{R}^4)$. So, for any $\lambda \in S^2$ we have a complex surface S_λ and a holomorphic bundle over S_λ . These data can be viewed in the following way. We consider the

projection $\pi: \mathbb{R}^4 \times S^2 \rightarrow \mathbb{R}^4$ and the pull-back $\pi^*(E)$ to $\mathbb{R}^4 \times S^2$. This pullback bundle has a connection which defines a holomorphic structure along each fiber $S_\lambda \subset \mathbb{R}^4 \times S^2$ of the other projection. The product $\mathbb{R}^4 \times S^2$ is the twistor space of \mathbb{R}^4 and it is in a natural way a three-dimensional complex manifold. It can be identified with the complement of a line L_∞ in \mathbb{CP}^3 where the projection $\mathbb{R}^4 \times S^2 \rightarrow S^2$ becomes the fibration of $\mathbb{CP}^3 \setminus L_\infty$ by the complex planes through L_∞ . One can see then that $\pi^*(E)$ is naturally a holomorphic bundle over $\mathbb{CP}^3 \setminus L_\infty$. The construction extends to the conformal compactification S^4 of \mathbb{R}^4 . If S^4 is viewed as the quaternionic projective line \mathbb{HP}^1 and we identify H^2 with \mathbb{C}^4 in the standard way, we get a natural map $\pi: \mathbb{CP}^3 \rightarrow \mathbb{HP}^1$. Then \mathbb{CP}^3 is the twistor space of S^4 and an anti-self-dual instanton on a bundle E over S^4 induces a holomorphic structure on the bundle $\pi^*(E)$ over \mathbb{CP}^3 .

In general, the twistor space Z of an oriented Riemannian 4-manifold M is defined to be the unit sphere bundle in Λ_M^+ . This has a natural almost-complex structure which is integrable if and only if the self-dual part of the Weyl curvature of M vanishes (Atiyah *et al.* 1978). The antipodal map on the 2-sphere induces an antiholomorphic involution of Z . In such a case, an anti-self-dual instanton over M lifts to a holomorphic bundle over Z . Conversely, a holomorphic bundle over Z which is holomorphically trivial over the fibers of the fibration $Z \rightarrow M$ (projective lines in Z), and which satisfies a certain reality condition with respect to the antipodal map, arises from a unitary instanton over M . This is the Ward correspondence, part of Penrose’s twistor theory.

The ADHM Construction

The problem of describing all solutions to the Yang–Mills instanton equation over S^4 is thus reduced to a problem in algebraic geometry, of classifying certain holomorphic vector bundles. This was solved by Atiyah *et al.* (1978). The resulting ADHM construction reduces the problem to certain matrix equations. The equations can be reduced to the following form. For a bundle Chern class k and rank r , we require a pair of $k \times k$ matrices α_1, α_2 , a $k \times r$ matrix a , and an $r \times k$ matrix b . Then the equations are

$$\begin{aligned} [\alpha_1, \alpha_2] &= ab \\ [\alpha_1^*, \alpha_1] + [\alpha_2^*, \alpha_2] &= aa^* - b^*b \end{aligned} \quad [1]$$

We also require certain open, nondegeneracy conditions. Given such matrix data, a holomorphic

bundle over \mathbb{CP}^3 is constructed via a “monad”: a pair of bundle maps over \mathbb{CP}^3

$$\begin{aligned} C^k \otimes \mathcal{O}(-1) @> D_1 >> C^k \oplus C^k \oplus C^r @> D_2 \\ >> C^k \otimes \mathcal{O}(1) \end{aligned}$$

with $D_2 D_1 = 0$. That is, the rank- r holomorphic bundle we construct is $\text{Ker } D_2 / \text{Im } D_1$. The bundle maps D_1, D_2 are obtained from the matrix data in a straightforward way, in suitable coordinates. It is this matrix description which was used by Boyer *et al.* to prove the Atiyah–Jones conjecture on the topology of the moduli spaces of instantons. The only other case when the twistor space of a compact 4-manifold is an algebraic variety is the complex projective plane, with the nonstandard orientation. An analog of the ADHM description in this case was given by Buchdahl (1986).

Integrable Systems

The Ward correspondence can be viewed in the general framework of integrable systems. Working with the standard complex structure on \mathbb{R}^4 , the integrability condition for the $\bar{\partial}$ -operator takes the shape

$$[\nabla_1 + i\nabla_2, \nabla_3 + i\nabla_4] = 0$$

where ∇_i are the components of the covariant derivative in the coordinate directions. So, the instanton equation can be viewed as a family of such commutator equations parametrized by $\lambda \in S^2$. One obtains many reductions of the instanton equation by imposing suitable symmetries. Solutions invariant under translation in one variable correspond to the Bogomolny “monopole equation” (Jaffe and Taubes 1980). Solutions invariant under three translations correspond to solutions of Nahm’s equations,

$$\frac{dT_i}{dt} = \epsilon_{ijk} [T_j, T_k]$$

for matrix-valued functions T_1, T_2, T_3 of one variable t . Nahm (1982) and Hitchin (1983) developed an analog of the ADHM construction relating these two equations. This is now seen as a part of a general “Fourier–Mukai–Nahm transform” (Donaldson and Kronheimer 1990). The instanton equations for connections invariant under two translations, Hitchin’s equations (Hitchin 1983), are locally equivalent to the harmonic map equation for a surface into the symmetric space dual to the structure group. Changing the signature of the metric on \mathbb{R}^4 to $(2, 2)$, one gets the harmonic mapping equations into Lie groups (Hitchin 1990). More complicated reductions yield almost all the known examples of

integrable PDEs as special forms of the instanton equations (Mason and Woodhouse 1996).

Moment Maps: the Kobayashi–Hitchin Conjecture

Let Σ be a compact Riemann surface. The Jacobian of Σ is the complex torus $H^1(\Sigma, \mathcal{O})/H^1(\Sigma, \mathbb{Z})$: it parametrizes holomorphic line bundles of degree 0 over Σ . The Hodge theory (which was, of course, developed long before Hodge in this case) shows that the Jacobian can also be identified with the torus $H^1(\Sigma, \mathbb{R})/H^1(\Sigma, \mathbb{Z})$ which parametrizes flat $U(1)$ -connections. That is, any holomorphic line bundle of degree 0 admits a unique compatible flat unitary connection.

The generalization of these ideas to bundles of higher rank began with Weil. He observed that any holomorphic vector bundle of degree 0 admits a flat connection, not necessarily unitary. Narasimhan and Seshadri (1965) showed that (in the case of degree 0) the existence of a flat, irreducible, unitary connection was equivalent to an algebro-geometric condition of stability which had been introduced shortly before by Mumford, for quite different purposes. Mumford introduced the stability condition in order to construct separated moduli spaces of holomorphic bundles – generalizing the Jacobian – as part of his general geometric invariant theory. For bundles of nonzero degree, the discussion is slightly modified by the use of projectively flat unitary connections. The result of Narasimhan and Seshadri asserts that there are two different descriptions of the same moduli space $\mathcal{M}^{d,r}(\Sigma)$: either as parametrizing certain irreducible projectively flat unitary connections (representations of $\pi_1(\Sigma)$), or parametrizing stable holomorphic bundles of degree d and rank r . While Narasimhan and Seshadri probably did not view the ideas in these terms, another formulation of their result is that a certain nonlinear PDE for a Hermitian metric on a holomorphic bundle – analogous to the Laplace equation in the abelian case – has a solution when the bundle is stable.

Atiyah and Bott (1982) cast these results in the framework of gauge theory. (The Yang–Mills equations in two dimensions essentially reduce to the condition that the connection be flat, so they are rather trivial locally but have interesting global structure.) They made the important observation that the curvature of a connection furnishes a map

$$F : \mathcal{A} \rightarrow \text{Lie}(\mathcal{G})^*$$

which is an equivariant moment map for the action of the gauge group on \mathcal{A} . Here the symplectic form on the affine space \mathcal{A} and the map from the adjoint

bundle-valued 2-forms to the dual of the Lie algebra of \mathcal{G} are both given by integration of products of forms. From this point of view, the Narasimhan–Seshadri result is an infinite-dimensional example of a general principle relating symplectic and complex quotients. At about the same time, Hitchin and Kobayashi independently proposed an extension of these ideas to higher dimensions. Let E be a holomorphic bundle over a complex manifold V . Any compatible unitary connection on E has curvature F of type $(1,1)$. Let ω be the $(1,1)$ -form corresponding to a fixed Hermitian metric on V . The Hermitian Yang–Mills equation is the equation

$$F \cdot \omega = \mu 1_E$$

where μ is a constant (determined by the topological invariant $c_1(E)$). The Kobayashi–Hitchin conjecture is that, when ω is Kähler, this equation has an irreducible solution if and only if E is a stable bundle in the sense of Mumford. Just as in the Riemann surface case, this equation can be viewed as a nonlinear second-order PDE of Laplace type for a metric on E . The moment map picture of Atiyah and Bott also extends to this higher-dimensional version. In the case when V has complex dimension 2 (and μ is zero), the Hermitian Yang–Mills connections are exactly the anti-self-dual instantons, so the conjecture asserts that the moduli spaces of instantons can be identified with certain moduli spaces of stable holomorphic bundles.

The Kobayashi–Hitchin conjecture was proved in the most general form by Uhlenbeck and Yau (1986), and in the case of algebraic manifolds in Donaldson (1987). The proofs in Donaldson (1985, 1987) developed some extra structure surrounding these equations, connected with the moment map point of view. The equations can be obtained as the Euler–Lagrange equations for a nonlocal functional, related to the renormalized determinants of Quillen and Bismut. The results have been extended to non-Kähler manifolds and certain noncompact manifolds. There are also many extensions to equations for systems of data comprising a bundle with additional structure such as a holomorphic section or Higgs’ field (Bradlow *et al.* 1995), or a parabolic structure along a divisor. Hitchin’s equations (Hitchin 1987) are a particularly rich example.

Topology of Moduli Spaces

The moduli spaces $\mathcal{M}_{r,d}(\Sigma)$ of stable holomorphic bundles/projectively flat unitary connections over Riemann surfaces Σ have been studied intensively from many points of view. They have natural Kähler structures: the complex structure being visible in the

holomorphic bundles guise and the symplectic form as the “Marsden–Weinstein quotient” in the unitary connections guise. In the case when r and d are coprime, they are compact manifolds with complicated topologies. There is an important basic construction for producing cohomology classes over these (and other) moduli spaces. One takes a universal bundle U over the product $\mathcal{M} \times \Sigma$ with Chern classes

$$c_i(U) \in H^{2i}(\mathcal{M} \times \Sigma)$$

Then, for any class $\alpha \in H_p(\Sigma)$, we get a cohomology class $c_i(U)/\alpha \in H^{2i-p}(\mathcal{M})$. Thus, if R_Σ is the graded ring freely generated by such classes, we have a homomorphism $\nu: R_\Sigma \rightarrow H^*(\mathcal{M})$. The questions about the topology of the moduli spaces which have been studied include:

1. finding the Betti numbers of the moduli space \mathcal{M} ;
2. identifying the kernel of ν ;
3. giving an explicit system of generators and relations for the ring $H^*(\mathcal{M})$;
4. identifying the Pontrayagin and Chern classes of \mathcal{M} within $H^*(\mathcal{M})$; and
5. evaluating the pairings

$$\int_{\mathcal{M}} \nu(W)$$

for elements W of the appropriate degree in R .

All of these questions have now been solved quite satisfactorily. In early work, Newstead (1967) found the Betti numbers in the rank-2 case. The main aim of Atiyah and Bott was to apply the ideas of Morse theory to the Yang–Mills functional over a Riemann surface and they were able to reproduce Newstead’s results in this way and extend them to higher rank. They also showed that the map ν is a surjection, so the universal bundle construction gives a system of generators for the cohomology. Newstead made conjectures on the vanishing of the Pontrayagin and Chern classes above a certain range which were established by Kirwan and extended to higher rank by Earl and Kirwan (1999). Knowing that R_Σ maps on to $H^*(\mathcal{M})$, a full set of relations can (by Poincaré duality) be deduced in principle from a knowledge of the integral pairings in (5) above, but this is not very explicit. A solution to (5) in the case of rank 2 was found by Thaddeus (1992). He used results from the Verlinde theory (see section on 3-manifolds below) and the Riemann–Roch formula. Another point of view was developed by Witten (1991), who showed that the volume of the moduli space was related to the theory of torsion in algebraic topology and satisfied simple gluing axioms. These different

points of view are compared in Donaldson (1993). Using a nonrigorous localization principle in infinite dimensions, Witten (1992) wrote down a general formula for the pairings (5) in any rank, and this was established rigorously by Jeffrey and Kirwan, using a finite-dimensional version of the same localization method. A very simple and explicit set of generators and relations for the cohomology (in the rank-2 case) was given by King and Newstead (1998). Finally, the quantum cohomology of the moduli space, in the rank-2 case, was identified explicitly by Munoz (1999).

Hyper-Kähler Quotients

Much of this story about the structure of moduli spaces extends to higher dimensions and to the moduli spaces of connections and Higgs fields. A particularly notable extension of the ideas involves hyper-Kähler structures. Let M be a hyper-Kähler 4-manifold, so there are three covariant-constant self-dual forms $\omega_1, \omega_2, \omega_3$ on M . These correspond to three complex structures I_1, I_2, I_3 obeying the algebra of the quaternions. If we single out one structure, say I_1 , the instantons on M can be viewed as holomorphic bundles with respect to I_1 satisfying the moment map condition (Hermitian Yang–Mills equation) defined by the form ω_1 . Taking a different complex structure interchanges the role of the moment map and integrability conditions. This can be put in a general framework of hyper-Kähler quotients due to Hitchin *et al.* (1987). Suppose initially that M is compact (so either a K3 surface or a torus). Then the ω_i components of the curvature define three maps

$$F_i : \mathcal{A} \rightarrow \text{Lie}(\mathcal{G})^*$$

The structures on M make \mathcal{A} into a flat hyper-Kähler manifold and the three maps F_i are the moment maps for the gauge group action with respect to the three symplectic forms on \mathcal{A} . In this situation, it is a general fact that the hyper-Kähler quotient – the quotient by \mathcal{G} of the common zero set of the three moment maps – has a natural hyper-Kähler structure. This hyper-Kähler quotient is just the moduli space of instantons over M . In the case when M is the noncompact manifold \mathbb{R}^4 , the same ideas apply except that one has to work with the based gauge group \mathcal{G}_0 . The conclusion is that the framed moduli spaces $\tilde{\mathcal{M}}$ of instantons over \mathbb{R}^4 are naturally hyper-Kähler manifolds. One can also see this hyper-Kähler structure through the ADHM matrix description. A variant of these matrix equations was used by Kronheimer to construct “gravitational instantons.” The same ideas also

apply to the moduli spaces of monopoles, where the hyper-Kähler metric, in the simplest case, was studied by Atiyah and Hitchin (1989).

Low-Dimensional Topology

Instantons and 4-Manifolds

Gauge theory has had unexpected applications in low-dimensional topology, particularly the topology of smooth 4-manifolds. The first work in this direction, in the early 1980s, involved the Yang–Mills instantons. The main issue in 4-manifold theory at that time was the correspondence between the diffeomorphism classification of simply connected 4-manifolds and the classification up to homotopy. The latter is determined by the intersection form, a unimodular quadratic form on the second integral homology group (i.e., a symmetric matrix with integral entries and determinant ± 1 , determined up to integral change of basis). The only known restriction was that Rohlin’s theorem, which asserts that if the form is even the signature must be divisible by 16. The achievement of the first phase of the theory was to show that

1. There are unimodular forms which satisfy the hypotheses of Rohlin’s theorem but which do not appear as the intersection forms of smooth 4-manifolds. In fact, no nonstandard definite form, such as a sum of copies of the E_8 matrix, can arise in this way.
2. There are simply connected smooth 4-manifolds which have isomorphic intersection forms, and hence are homotopy equivalent, but which are not diffeomorphic.

These results stand in contrast to the homeomorphism classification which was obtained by Freedman shortly before and which is almost the same as the homotopy classification.

The original proof of item (1) above argued with the moduli space \mathcal{M} of anti-self-dual instantons $\text{SU}(2)$ instantons on a bundle with $c_2 = 1$ over a simply connected Riemannian 4-manifold M with a negative-definite intersection form (Donaldson 1983). In the model case when M is the 4-sphere the moduli space \mathcal{M} can be identified explicitly with the open 5-ball. Thus the 4-sphere arises as the natural boundary of the moduli space. A sequence of points in the moduli space converging to a boundary point corresponds to a sequence of connections with curvature densities converging to a δ -function, as described earlier. One shows that in the general case (under our hypotheses on the 4-manifold M) the moduli space \mathcal{M} has a similar behavior, it contains a collar $M \times (0, \delta)$

formed by instantons made using Taubes' gluing construction, described previously. The complement of this collar is compact. In the interior of the moduli space, there are a finite number of special points corresponding to $U(1)$ -reductions of the bundle P . This is the way in which the moduli space "sees" the integral structure of the intersection form since such reductions correspond to integral homology classes with self-intersection -1 . Neighborhoods of these special points are modeled on quotients $\mathbb{C}^3/U(1)$; that is, cones on copies of \mathbb{CP}^2 . The upshot is that (for generic Riemannian metrics on M) the moduli space gives a cobordism from the manifold M to a set of copies of \mathbb{CP}^2 which can be counted in terms of the intersection form, and the result follows easily from standard topology. More sophisticated versions of the argument extended the results to rule out some indefinite intersection forms.

On the other hand, the original proofs of item (2) used "invariants" defined by instanton moduli spaces (Donaldson 1990). The general scheme exploits the same construction outlined in the previous section. We suppose that M is a simply connected 4-manifold with $b^+(M) = 1 + 2p$, where $p > 0$ is an integer. (Here $b^+(M)$ is, as usual, the number of positive eigenvalues of the intersection matrix.) Ignoring some technical restrictions, there is a map

$$\nu: R_M \rightarrow H^*(\mathcal{M}_k)$$

where R_M is a graded ring freely generated by the homology (below the top dimension) of the 4-manifold M and \mathcal{M}_k is the moduli space of anti-self-dual $SU(2)$ -instantons on a bundle with $c_2 = k > 0$. For an element W in R_M of the appropriate degree, one obtains a number by evaluating, or integrating, $\nu(W)$ on \mathcal{M}_k . The main technical difficulty here is that the moduli space \mathcal{M}_k is rarely compact, so one needs to make sense of this "evaluation." With all the appropriate technicalities in place, these invariants could be shown to distinguish various homotopy-equivalent, homeomorphic 4-manifolds. All these early developments are described in detail in the book by Donaldson and Kronheimer (1990).

Basic Classes

Until the early 1990s, these instanton invariants could only be calculated in isolated favorable cases (although the calculations which were made, through the work of many mathematicians, led to a large number of further results about 4-manifold topology). Deeper understanding of their structure came with the work of Kronheimer and Mrowka. This work was, in large part,

motivated by a natural question in geometric topology. Any homology class $\alpha \in H_2(M; \mathbb{Z})$ can be represented by an embedded, connected, smooth surface. One can define an integer $g(\alpha)$ to be the minimal genus of such a representative. The problem is to find $g(\alpha)$, or at least bounds on it. A well-known conjecture, ascribed to Thom, was that when M is the complex projective plane the minimal genus is realized by a complex curve; that is,

$$g(\pm dH) = \frac{1}{2}(d-1)(d-2)$$

where H is the standard generator of $H_2(\mathbb{CP}^2)$ and $d \geq 1$.

The new geometrical idea introduced by Kronheimer and Mrowka was to study instantons over a 4-manifold M with singularities along a surface $\Sigma \subset M$. For such connections, there is a real parameter: the limit of the trace of the holonomy around small circles linking the surface. By varying this parameter, they were able to interpolate between moduli spaces of nonsingular instantons on different bundles over M and obtain relations between the different invariants. They also found that if the genus of Σ is suitably small then some of the invariants are forced to vanish, thus, conversely, getting information about g for 4-manifolds with nontrivial invariants. For example, they showed that if M is a K3 surface then $g(\alpha) = (1/2)(\alpha \cdot \alpha + 2)$.

The structural results of Kronheimer and Mrowka (1995) introduced the notion of a 4-manifold of "simple type." Write the invariant defined above by the moduli space \mathcal{M}_k as $I_k: R_M \rightarrow \mathbb{Q}$. Then I_k vanishes except on terms of degree $2d(k)$, where $d(k) = 4k - 3(1+p)$. We can put all these together to define $\underline{I} = \sum I_k: R_M \rightarrow \mathbb{Q}$. The ring R_M is a polynomial ring generated by classes $\alpha \in H_2(M)$, which have degree 2 in R_M , and a class X of degree 4 in R_M , corresponding to the generator of $H_0(M)$. The 4-manifold is of simple type if

$$\underline{I}(X^2 W) = 4\underline{I}(W)$$

for all $W \in R_M$. Under this condition, Kronheimer and Mrowka showed that all the invariants are determined by a finite set of "basic" classes $K_1, \dots, K_s \in H_2(M)$ and rational numbers β_1, \dots, β_s . To express the relation, they form a generating function

$$\mathcal{D}_M(\alpha) = \underline{I}(e^\alpha) + \underline{I}\left(\frac{X}{2}e^\alpha\right)$$

This is *a priori* a formal power series in $H^2(M)$ but *a posteriori* the series converges and can be regarded

as a function on $H_2(M)$. Kronheimer and Mrowka's result is that

$$\mathcal{D}_M(\alpha) = \exp\left(\frac{\alpha \cdot \alpha}{2}\right) \sum_{r=1}^s \beta_r e^{K_r \cdot \alpha}$$

It is not known whether all simply connected 4-manifolds are of simple type, but Kronheimer and Mrowka were able to show that this is the case for a multitude of examples. They also introduced a weaker notion of "finite type," and this condition was shown to hold in general by Munoz and Froyshov. The overall result of this work of Kronheimer and Mrowka was to make the calculation of the instanton invariants for many familiar 4-manifolds a comparatively straightforward matter.

3-Manifolds: Casson's Invariant

Gauge theory has also entered into 3-manifold topology. In 1985, Casson introduced a new integer-valued invariant of oriented homology 3-spheres which "counts" the set Z of equivalence classes of irreducible flat $SU(2)$ -connections, or equivalently irreducible representations $\pi_1(Y) \rightarrow SU(2)$. Casson's approach (Akbulut and McCarthy 1990) was to use a Heegard splitting of a 3-manifold Y into two handle bodies Y^+, Y^- with a surface Σ as common boundary. Then $\pi_1(\Sigma)$ maps onto $\pi_1(Y)$ and a flat $SU(2)$ connection on Y is determined by its restriction to Σ . Let M_Σ be the moduli space of irreducible flat connections over Σ (as discussed in the last section) and let $L^\pm \subset M_\Sigma$ be the subsets which extend over Y^\pm . Then L^\pm are submanifolds of half the dimension of M_Σ and the set Z can be identified with the intersection $L^+ \cap L^-$. The Casson invariant is one-half the algebraic intersection number of L^+ and L^- . Casson showed that this is independent of the Heegard splitting (and is also, in fact, an integer, although this is not obvious). He showed that when Y is changed by Dehn surgery along a knot, the invariant changes by a term computed from the Alexander polynomial of the knot. This makes the Casson invariant computable in examples. (For a discussion of Casson's formula see Donaldson (1999).) Taubes showed that the Casson invariant could also be obtained in a more differential-geometric fashion, analogous to the instanton invariants of 4-manifolds (Taubes 1990).

3-Manifolds: Floer Theory

Independently, at about the same time, Floer (1989) introduced more sophisticated invariants – the Floer homology groups – of homology 3-spheres, using gauge theory. This development

ran parallel to his introduction of similar ideas in symplectic geometry. Suppose, for simplicity, that the set Z of equivalence classes of irreducible flat connections is finite. For pairs ρ_-, ρ_+ in Z , Floer considered the instantons on the tube $Y \times \mathbb{R}$ asymptotic to ρ^\pm at $\pm\infty$. There is an infinite set of moduli spaces of such instantons, labeled by a relative Chern class, but the dimensions of these moduli spaces agree modulo 8. This gives a relative index $\delta(\rho_-, \rho_+) \in \mathbb{Z}/8$. If $\delta(\rho_-, \rho_+) = 1$ there is a moduli space of dimension 1 (possibly empty), but the translations of the tube act on this moduli space and, dividing by translations, we get a finite set. The number of points in this set, counted with suitable signs, gives an integer $n(\rho_-, \rho_+)$. Then, Floer considers the free abelian groups

$$C_* = \bigoplus_{\rho \in Z} \mathbb{Z}\langle \rho \rangle$$

generated by the set Z and a map $\partial: C_* \rightarrow C_*$ defined by

$$\partial(\langle \rho_- \rangle) = \sum n(\rho_-, \rho_+) \langle \rho_+ \rangle$$

Here the sum runs over the ρ_+ with $\delta(\rho_-, \rho_+) = 1$. Floer showed that $\partial^2 = 0$ and the homology $HF_*(Y) = \ker \partial / \text{Im } \partial$ is independent of the metric on Y (and various other choices made in implementing the construction in detail). The chain complex C_* and hence the Floer homology can be graded by $\mathbb{Z}/8$, using the relative index, so the upshot is to define 8 abelian groups $HF_i(Y)$: invariants of the 3-manifold Y . The Casson invariant appears now as the Euler characteristic of the Floer homology. There has been extensive work on extending these ideas to other 3-manifolds (not homology spheres) and gauge groups, but this line of research does not yet seem to have reached a clear-cut conclusion.

Part of the motivation for Floer's work came from Morse theory, and particularly the approach to this theory expounded by Witten (1982). The Chern–Simons functional is a map

$$CS: \mathcal{A}/\mathcal{G} \rightarrow \mathbb{R}/\mathbb{Z}$$

from the space of $SU(2)$ -connections over Y . Explicitly, in a trivialization of the bundle

$$CS(A) = \int_Y A \wedge dA + \frac{3}{2} A \wedge A \wedge A$$

It appears as a boundary term in the Chern–Weil theory for the second Chern class, in a similar way as holonomy appears as a boundary term in the Gauss–Bonnet theorem. The set Z can be identified with the critical points of CS and the instantons on the tube as integral curves of the gradient vector

field of CS. Floer's definition mimics the definition of homology in ordinary Morse theory, taking Witten's point of view. It can be regarded formally as the "middle-dimensional" homology of the infinite-dimensional space \mathcal{A}/\mathcal{G} . See Atiyah (1988) and Cohen *et al.* (1995) for discussions of these ideas.

The Floer theory interacts with 4-manifold invariants, making up a structure approximating to a $(3+1)$ -dimensional topological field theory (Atiyah 1988). Roughly, the numerical invariants of closed 4-manifolds generalize to invariants for a 4-manifold M with boundary Y taking values in the Floer homology of Y . If two such manifolds are glued along a common boundary, the invariants of the result are obtained by a pairing in the Floer groups. There are, however, at the moment, some substantial technical restrictions on this picture. This theory, as well as Floer's original construction, is developed in detail by Donaldson (2002). At the time of writing, the Floer homology groups are still difficult to compute in examples. One important tool is a surgery-exact sequence found by Floer (Braam and Donaldson 1995), related to Casson's surgery formula.

3-Manifolds: Jones–Witten Theory

There is another, quite different, way in which ideas from gauge theory have entered 3-manifold topology. This is the Jones–Witten theory of knot and 3-manifold invariants. This theory falls outside the main line of this article, but we will say a little about it since it draws on many of the ideas we have discussed. The goal of the theory is to construct a family of $(2+1)$ -dimensional topological field theories indexed by an integer k , assigning complex vector space $H_k(\Sigma)$ to a surface Σ and an invariant in $H_k(\partial Y)$ to a 3-manifold-with-boundary Y . If ∂Y is empty, the vector space $H_k(\partial Y)$ is taken to be \mathbb{C} , so one seeks numerical invariants of closed 3-manifolds. Witten's (1989) idea is that these invariants of closed 3-manifolds are Feynmann integrals

$$\int_{\mathcal{A}/\mathcal{G}} e^{i2\pi k \text{CS}(A)} \mathcal{D}A$$

This functional integral is probably a schematic rather than a rigorous notion. The data associated with surfaces can, however, be defined rigorously. If we fix a complex structure I on Σ , we can define a vector space $H_k(\Sigma, I)$ to be

$$H_k(\Sigma, I) = H^0(\mathcal{M}(\Sigma); L^k)$$

where $\mathcal{M}(\Sigma)$ is the moduli space of stable holomorphic bundles/flat unitary connections over Σ and L is a certain holomorphic line bundle over

$\mathcal{M}(\Sigma)$. These are the spaces of "conformal blocks" whose dimension is given by the Verlinde formulas. Recall that $\mathcal{M}(\Sigma)$, as a symplectic manifold, is canonically associated with the surface Σ , without any choice of complex structure. The Hilbert spaces $H_k(\Sigma, I)$ can be regarded as the quantization of this symplectic manifold, in the general framework of geometric quantization: the inverse of k plays the role of Planck's constant. What is not obvious is that this quantization is independent of the complex structure chosen on the Riemann surface: that is, that there is a natural identification of the vector spaces (or at least the associated projective spaces) formed by using different complex structures. This was established rigorously by Hitchin (1990) and Axelrod *et al.* (1991), who constructed a projectively flat connection on the bundle of spaces $H_k(\Sigma, I)$ over the space of complex structures I on Σ . At a formal level, these constructions are derived from the construction of the metaplectic representation of a linear symplectic group, since the \mathcal{M}_Σ are symplectic quotients of an affine symplectic space.

The Jones–Witten invariants have been rigorously established by indirect means, but it seems that there is still work to be done in developing Witten's point of view. If Y^+ is a 3-manifold with boundary, one would like to have a geometric definition of a vector in $H_k(\partial Y^+)$. This should be the quantized version of the submanifold L^+ (which is Lagrangian in \mathcal{M}_Σ) entering into the Casson theory.

Seiberg–Witten Invariants

The instanton invariants of a 4-manifold can be regarded as the integrals of certain natural differential forms over the moduli spaces of instantons. Witten (1988) showed that these invariants could be obtained as functional integrals, involving a variant of the Feynman integral, over the space of connections and certain auxiliary fields (insofar as this latter integral is defined at all). A geometric explanation of Witten's construction was given by Atiyah and Jeffrey (1990). Developing this point of view, Witten made a series of predictions about the instanton invariants, many of which were subsequently verified by other means. This line of work culminated in 1994 where, applying developments in supersymmetric Yang–Mills QFT, Seiberg and Witten introduced a new system of invariants and a precise prediction as to how these should be related to the earlier ones.

The Seiberg–Witten invariants (Witten 1994) are associated with a Spin^c structure on a 4-manifold M . If M is simply connected this is specified by a class $K \in H^2(M; \mathbb{Z})$ lifting $w_2(M)$. One has spin bundles

$S^+, S^- \rightarrow M$ with $c_1(S^\pm) = K$. The Seiberg–Witten equation is for a spinor field ϕ – a section of S^+ and a connection A on the complex line bundle $\Lambda^2 S^+$. This gives a connection on S^+ and hence a Dirac operator

$$D_A : \Gamma(S^+) \rightarrow \Gamma(S^-)$$

The Seiberg–Witten equations are

$$D_A \phi = 0, \quad F_A^+ = \sigma(\phi)$$

where $\sigma : S^+ \rightarrow \Lambda^+$ is a certain natural quadratic map. The crucial differential-geometric feature of these equations arises from the Weitzenböck formula

$$D_A^* D_A \phi = \nabla_A^* \nabla_A \phi + \frac{R}{4} \phi + \rho(F^+) \phi$$

where R is the scalar curvature and ρ is a natural map from Λ^+ to the endomorphisms of S^+ . Then ρ is adjoint to σ and

$$\langle \rho(\sigma(\phi)) \phi, \phi \rangle = |\phi|^4$$

It follows easily from this that the moduli space of solutions to the Seiberg–Witten equation is compact. The most important invariants arise when K is chosen so that

$$K \cdot K = 2\chi(M) + 3 \operatorname{sign}(M)$$

where $\chi(M)$ is the Euler characteristic and $\operatorname{sign}(M)$ is the signature. (This is just the condition for K to correspond to an almost-complex structure on M .) In this case, the moduli space of solutions is zero dimensional (after generic perturbation) and the Seiberg–Witten invariant $\operatorname{SW}(K)$ is the number of points in the moduli space, counted with suitable signs.

Witten’s conjecture relating the invariants, in its simplest form, is that when M has simple type the classes K for which $\operatorname{SW}(K)$ is nonzero are exactly the basic classes K_r of Kronheimer and Mrowka and that

$$\beta_r = 2^{C(M)} \operatorname{SW}(K_r)$$

where $C(M) = 2 + (1/4)(7\chi(M) + 11 \operatorname{sign}(M))$. This asserts that the two sets of invariants contain exactly the same information about the 4-manifold.

The evidence for this conjecture, via calculations of examples, is very strong. A somewhat weaker statement has been proved rigorously by Feehan and Leness (2003). They use an approach suggested by Pidstragatch and Tyurin, studying moduli spaces of solutions to a nonabelian version of the Seiberg–Witten equations. These contain both the instanton and abelian Seiberg–Witten moduli spaces, and the strategy is to relate the topology of these two sets by standard localization arguments. (This approach is related to ideas introduced by Thaddeus (1994) in the

case of bundles over Riemann surfaces.) The serious technical difficulty in this approach stems from the lack of compactness of the nonabelian moduli spaces. The more general versions of Witten’s conjecture (Moore and Witten 1997) (e.g., when $b^+(M) = 1$) contain very complicated formulas, involving modular forms, which presumably arise as contributions from the compactification of the moduli spaces.

Applications

Regardless of the connection with the instanton theory, one can go ahead directly to apply the Seiberg–Witten invariants to 4-manifold topology, and this has been the main direction of research since the 1990s. The features of the Seiberg–Witten theory which have led to the most prominent developments are the following.

1. The reduction of the equations to two dimensions is very easy to understand. This has led to proofs of the Thom conjecture and wide-ranging generalizations (Ozsvath and Szabo 2000).
2. The Weitzenböck formula implies that, if M has positive scalar curvature, then solutions to the Seiberg–Witten equations must have $\phi = 0$. This has led to important interactions with four-dimensional Riemannian geometry (Lebrun 1996).
3. In the case when M is a symplectic manifold, there is a natural deformation of the Seiberg–Witten equations, discovered by Taubes (1996), who used it to show that the Seiberg–Witten invariants of M are nontrivial. More generally, Taubes showed that for large values of the deformation parameter the solutions of the deformed equation localize around surfaces in the 4-manifold and used this to relate the Seiberg–Witten invariants to the Gromov theory of pseudoholomorphic curves. These results of Taubes have completely transformed the subject of four-dimensional symplectic geometry.

Bauer and Furuta (2004) have combined the Seiberg–Witten theory with more sophisticated algebraic topology to obtain further results about 4-manifolds. They consider the map from the space of connections and spinor fields defined by the formulas on the left-hand side of the equations. The general idea is to obtain invariants from the homotopy class of this map, under a suitable notion of homotopy. A technical complication arises from the gauge group action, but this can be reduced to the action of a single $U(1)$. Ignoring this issue, Bauer and Furuta have obtained invariants in the stable homotopy groups $\lim_{N \rightarrow \infty} \pi_{N+r}(S^N)$, which reduce to the ordinary numerical invariants when $r = 1$. Using these invariants, they obtain results about connected sums of

4-manifolds, for which the ordinary invariants are trivial. Using refined cobordism invariants ideas, Furuta made great progress towards resolving the question of which intersection forms arise from smooth, simply connected 4-manifolds. A well-known conjecture is that, if such a manifold is spin, then the second Betti number satisfies

$$b_2(M) \geq \frac{11}{8} |\text{sign}(M)|$$

Furuta (2001) proved that $b_2(M) \geq (10/8)|\text{sign}(M)| + 2$.

An important and very recent achievement, bringing together many different lines of work, is the proof of “Property P” in 3-manifold topology by Kronheimer and Mrowka (2004). This asserts that one cannot obtain a homotopy sphere (counter-example to the Poincaré conjecture) by +1-surgery along a nontrivial knot in S^3 . The proof uses work of Gabai and Eliashberg to show that the manifold obtained by 0-framed surgery is embedded in a symplectic 4-manifold; Taubes’ results to show that the Seiberg–Witten invariants of this 4-manifold are nontrivial; Feehan and Leness’ partial proof of Witten’s conjecture to show that the same is true for the instanton invariants; and the gluing rule and Floer’s exact sequence to show that the Floer homology of the +1-surgered manifold is nontrivial. It follows then from the definition of Floer homology that the fundamental group of this manifold is not trivial; in fact, it must have an irreducible representation in $SU(2)$.

See also: Cotangent Bundle Reduction; Floer Homology; Gauge Theories from Strings; Gauge Theoretic Invariants of 4-Manifolds; Instantons: Topological Aspects; Knot Homologies; Moduli Spaces: An Introduction; Nonperturbative and Topological Aspects of Gauge Theory; Seiberg–Witten Theory; Topological Quantum Field Theory: Overview; Variational Techniques for Ginzburg–Landau Energies.

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General Relativity: Experimental Tests

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Introduction

Einstein’s general theory of relativity has become the foundation for our understanding of the gravitational interaction. Four decades of high-precision

experiments have verified the theory with ever-increasing precision, with no confirmed evidence of a deviation from its predictions. The theory is now the standard framework for much of astronomy, with its searches for black holes, neutron stars, gravitational waves, and the origin and fate of the universe.

Yet modern developments in particle theory suggest that it may not be the entire story, and that

modification of the basic theory may be required at some level. String theory generally predicts a proliferation of gravity-like fields that could result in alterations of general relativity (GR) reminiscent of the Brans–Dicke theory of the 1960s. In the presence of extra dimensions, the gravity of the four-dimensional “brane” of a higher-dimensional world could be somewhat different from a pure four-dimensional GR. However, any theoretical speculation along these lines must still abide by the best current empirical bounds. This article will review experimental tests of GR and the theoretical implications of the results.

The Einstein Equivalence Principle

The Einstein equivalence principle is a modern generalization of Einstein’s 1907 idea of an equivalence between gravity and acceleration, or between free fall and an absence of gravity. It states that: (1) test bodies fall with the same acceleration independently of their internal structure or composition (weak equivalence principle, or WEP); (2) the outcome of any local nongravitational experiment is independent of the velocity of the freely falling reference frame in which it is performed (local Lorentz invariance, or LLI); and (3) the outcome of any local nongravitational experiment is independent of where and when in the universe it is performed (local position invariance, or LPI).

This principle is fundamental to gravitational theory, for it is possible to argue that, if EEP is valid, then gravitation and geometry are synonymous. In other words, gravity must be described by a “metric theory of gravity,” in which (1) spacetime is endowed with a symmetric metric, (2) the trajectories of freely falling bodies are geodesics of that metric, and (3) in local freely falling reference frames, the nongravitational laws of physics are those written in the language of special relativity (see Will (1993) for further details).

GR is a metric theory of gravity, but so are many others, including the scalar–tensor theory of Brans and Dicke and many of its modern descendents, some of which are inspired by string theory.

Tests of the Weak Equivalence Principle

To test the WEP, one compares the acceleration of two laboratory-sized bodies of different composition in an external gravitational field. Although legend suggests that Galileo may have demonstrated this principle to his students at the Leaning Tower of Pisa, and Newton tested it by means of pendulum experiments, the first true high-precision experiments

were done at the end of the nineteenth century by the Hungarian physicist Baron Roland von Eötvös and colleagues.

Eötvös employed a torsion balance, in which (schematically) two bodies of different composition are suspended at the ends of a rod that is supported horizontally by a fine wire or fiber. One then looks for a difference in the horizontal accelerations of the two bodies as revealed by a slight rotation of the rod. The source of the horizontal gravitational force could be the Sun, a large mass in or near the laboratory, or, as Eötvös recognized, the Earth itself. A measurement or limit on the fractional difference in acceleration between two bodies yields a quantity $\eta \equiv 2|a_1 - a_2|/|a_1 + a_2|$, called the “Eötvös ratio.” Eötvös’ experiments showed that η was smaller than a few parts in 10^9 , and later classic experiments in the 1960s and 1970s by Dicke and Braginsky improved the bounds by several orders of magnitude. Additional experiments were carried out during the 1980s as part of a search for a putative “fifth force,” that was motivated in part by a re-analysis of Eötvös’ original data.

The best limit on η currently comes from experiments carried out during the 1985–2000 period at the University of Washington (called the “Eöt-Wash” experiments), which used a sophisticated torsion balance tray to compare the accelerations of bodies of different composition toward the Earth, the Sun, and the galaxy. Another strong bound comes from ongoing laser ranging to reflectors deposited on the Moon during the Apollo program in the 1970s (lunar laser ranging, LLR), which routinely determines the Earth–Moon distance to millimeter accuracies. The data may be used to check the equality of acceleration of the Earth and Moon toward the Sun. The results from laboratory and LLR experiments are (Will 2001):

$$\eta_{\text{Eöt-Wash}} < 4 \times 10^{-13}, \quad \eta_{\text{LLR}} < 5 \times 10^{-13} \quad [1]$$

LLR also shows that gravitational binding energy falls with the same acceleration as ordinary matter to 1.3×10^{-3} (test of the Nordtvedt effect – see the section “Bounds on the PPN parameters” and Table 1).

Many of the high-precision, low-noise methods that were developed for tests of WEP have been adapted to laboratory tests of the inverse-square law of Newtonian gravitation at millimeter scales and below. The goal of these experiments is to search for additional gravitational interactions involving massive particles or for the presence of large extra dimensions. The challenge of these experiments is to distinguish gravitation-like interactions from electromagnetic and quantum-mechanical effects. No deviations from

Table 1 Current limits on the PPN parameters

Parameter	Effect	Limit	Remarks
$\gamma - 1$	(i) Shapiro delay	2.3×10^{-5}	Cassini tracking
	(ii) Light deflection	4×10^{-4}	VLBI
$\beta - 1$	(i) Perihelion shift	3×10^{-3}	$J_2 = 10^{-7}$ from helioseismology
	(ii) Nordtvedt effect	2.3×10^{-4}	LLR plus bounds on other parameters
ξ	Anisotropy in Newton's G	10^{-3}	Gravimeter bounds on anomalous Earth tides
α_1	Orbit polarization for moving systems	10^{-4}	Lunar laser ranging
α_2	Anomalous spin precession for moving bodies	4×10^{-7}	Alignment of solar axis relative to ecliptic
α_3	Anomalous self-acceleration for spinning moving bodies	2×10^{-20}	Pulsar spindown timing data
η^a	Nordtvedt effect	9×10^{-4}	Lunar laser ranging
ζ_1		2×10^{-2}	Combined PPN bounds
ζ_2	Anomalous self-acceleration for binary systems	4×10^{-5}	Timing data for PSR 1913 + 16
ζ_3	Violation of Newton's third law	10^{-8}	Lunar laser ranging
ζ_4			Not independent

^aHere $\eta = 4\beta - \gamma - 3 - 10\xi/3 - \alpha_1 + 2\alpha_2/3 - 2\zeta_1/3 - \zeta_2/3$.

Newton's inverse-square law have been found to date at distances between 10 μ m and 10 mm.

Tests of Local Lorentz Invariance

Although special relativity itself never benefited from the kind of "crucial" experiments, such as the perihelion advance of Mercury and the deflection of light, that contributed so much to the initial acceptance of GR and to the fame of Einstein, the steady accumulation of experimental support, together with the successful integration of special relativity into quantum mechanics, led to its being accepted by mainstream physicists by the late 1920s, ultimately to become part of the standard toolkit of every working physicist.

But in recent years new experiments have placed very tight bounds on any violations of the Lorentz invariance, which underlies special relativity. A simple way of interpreting this new class of experiments is to suppose that a coupling of some external gravitation-like field (not the metric) to the electromagnetic interactions results in an effective change in the speed of electromagnetic radiation, c , relative to the limiting speed of material test particles, c_0 ; in other words, $c \neq c_0$. It can be shown that such a Lorentz-noninvariant electromagnetic interaction would cause shifts in the energy levels of atoms and nuclei that depend on the orientation of the quantization axis of the state relative to our velocity relative to the rest of the universe, and on the quantum numbers of the state, resulting in orientation dependences of the fundamental frequencies of such atomic clocks. The magnitude of these "clock anisotropies" would be proportional to $\delta \equiv |(c_0/c)^2 - 1|$, which vanishes if Lorentz invariance holds (see Will (1993) and Haugan and Will (1987) for details).

The earliest clock anisotropy experiments were carried out around 1960 independently by Hughes and Drever, although their original motivation was somewhat different. Dramatic improvements were made in the 1980s using laser-cooled trapped atoms and ions. This technique made it possible to reduce the broadening of resonance lines caused by collisions, leading to the impressive bound $|\delta| > 10^{-21}$ (Will 2001).

Other recent tests of Lorentz invariance violation include comparisons of resonant cavities with atomic clocks, tests of dispersion and birefringence in the propagation of high-energy photons from astrophysical sources, threshold effects in elementary particle collisions, and anomalies in neutrino oscillations. Mattingly (2005) gives a thorough and up-to-date review of both the theoretical frameworks for studying these effects and the experimental results.

Tests of Local Position Invariance

LPI requires, among other things, that the internal binding energies of atoms and nuclei be independent of location in space and time, when measured against some standard atom. This means that a comparison of the rates of two different kinds of atomic clocks should be independent of location or epoch, and that the frequency shift between two identical clocks at different locations is simply a consequence of the apparent Doppler shift between a pair of inertial frames momentarily comoving with the clocks at the moments of emission and reception, respectively. The relevant parameter α appears in the formula for the frequency shift,

$$\Delta f/f = (1 + \alpha)\Delta\Phi/c^2$$

[2]

where Φ is the Newtonian gravitational potential. If LPI holds, $\alpha=0$. An early test of this was the Pound–Rebka experiment of 1960, which measured the frequency shift of gamma rays from radioactive iron nuclei in a tower at Harvard University. The best bounds come from a 1976 experiment in which a hydrogen maser atomic clock was launched to 10 000 km altitude on a Scout rocket and its frequency compared via telemetry with an identical clock on the ground, and a 1993 experiment in which two different kinds of atomic clocks were intercompared as a function of the varying solar gravitational field as seen on Earth (a “null” redshift experiment). The results are (Will 2001):

$$\alpha_{\text{Maser}} < 2 \times 10^{-4}, \quad \alpha_{\text{Null}} < 10^{-3} \quad [3]$$

Recent “clock comparison” tests of LPI include experiments done at the National Institute of Standards and Technology (NIST) in Boulder and at the Observatory of Paris, to look for cosmological variations in clock rates. The NIST experiment compared laser-cooled mercury ions with neutral cesium atoms over a two-year period, while the Paris experiment compared laser-cooled cesium and rubidium atomic fountains over five years; the results showed that the fine-structure constant is constant in time to a part in 10^{15} per year. A better bound of $6 \times 10^{-17} \text{ yr}^{-1}$ comes from analysis of fission yields of the Oklo natural reactor, which occurred in Africa two billion years ago.

Solar-System Tests

The Parametrized Post-Newtonian Framework

It was once customary to discuss experimental tests of GR in terms of the “three classical tests,” the gravitational redshift (which is really a test of the EEP, not of GR itself; see the section on tests of LPI), the perihelion advance of Mercury (the first success of the theory), and the deflection of light (whose measurement in 1919 made Einstein a celebrity). However, the proliferation of additional experimental tests and of well-motivated alternative metric theories of gravity made it desirable to develop a more general theoretical framework for analyzing both experiments and theories. This “parametrized post-Newtonian (PPN) framework” dates back to Eddington in 1922, but was fully developed by Nordtvedt and Will in the period 1968–72 (see Will (1993) for details).

When attention is confined to metric theories of gravity and, further, the focus is on the slow-motion, weak-field limit appropriate to the solar system and similar systems, it turns out that, in a broad class of metric theories, only the numerical values of a set of

coefficients in the spacetime metric vary from theory to theory. The resulting PPN framework contains ten parameters: γ , related to the amount of spatial curvature generated by mass; β , related to the degree of nonlinearity in the gravitational field; ξ , α_1 , α_2 , and α_3 , which determine whether the theory violates LPI or LLI in gravitational experiments; and ζ_1 , ζ_2 , ζ_3 , and ζ_4 , which describe whether the theory has appropriate momentum conservation laws. In GR, $\gamma=1$, $\beta=1$, and the remaining parameters all vanish. In the scalar-tensor theory of Brans–Dicke, $\gamma=(1+\omega_{\text{BD}})/(2+\omega_{\text{BD}})$, where ω_{BD} is an adjustable parameter.

A number of well-known relativistic effects can be expressed in terms of these PPN parameters:

Deflection of light

$$\begin{aligned} \Delta\theta &= \left(\frac{1+\gamma}{2}\right) \frac{4GM}{dc^2} \\ &= \left(\frac{1+\gamma}{2}\right) \times 1.7505 \frac{R_{\odot}}{d} \text{ arcsec} \end{aligned} \quad [4]$$

where d is the distance of closest approach of a ray of light to a body of mass M , and where the second line is the deflection by the Sun, with radius R_{\odot} .

Shapiro time delay

$$\Delta t = \left(\frac{1+\gamma}{2}\right) \frac{4GM}{c^3} \ln \left[\frac{(r_1 + \mathbf{x}_1 \cdot \mathbf{n})(r_2 - \mathbf{x}_2 \cdot \mathbf{n})}{d^2} \right] \quad [5]$$

where Δt is the excess travel time of a round-trip electromagnetic tracking signal, \mathbf{x}_1 and \mathbf{x}_2 are the locations relative to the body of mass M of the emitter and receiver of the round-trip signal (r_1 and r_2 are the respective distances), and \mathbf{n} is the direction of the outgoing tracking signal.

Perihelion advance

$$\begin{aligned} \frac{d\omega}{dt} &= \left(\frac{2+2\gamma-\beta}{3}\right) \frac{GM}{Pa(1-e^2)c^2} \\ &= \left(\frac{2+2\gamma-\beta}{3}\right) \times 42.98 \text{ arcsec}/100 \text{ yr} \end{aligned} \quad [6]$$

where P , a , and e are the period, semimajor axis, and eccentricity of the planet’s orbit, respectively; the second line is the value for Mercury.

Nordtvedt effect

$$\begin{aligned} \frac{m_G - m_I}{m_I} &= \left(4\beta - \gamma - 3 - \frac{10}{3}\xi - \alpha_1 + \frac{2}{3}\alpha_2 \right. \\ &\quad \left. - \frac{2}{3}\zeta_1 - \frac{1}{3}\zeta_2\right) \frac{|E_g|}{m_I c^2} \end{aligned} \quad [7]$$

where m_G and m_I are, respectively, the gravitational and inertial masses of a body such as the Earth or

Moon, and E_g is its gravitational binding energy. A nonzero Nordtvedt effect would cause the Earth and Moon to fall with a different acceleration toward the Sun. In GR, this effect vanishes.

Precession of a gyroscope

$$\begin{aligned}\frac{dS}{dt} &= (\Omega_{\text{FD}} + \Omega_{\text{Geo}}) \times S \\ \Omega_{\text{FD}} &= -\frac{1}{2} \left(1 + \gamma + \frac{\alpha_1}{4} \right) \frac{G}{r^3 c^2} (\mathbf{J} - 3 \mathbf{n} \mathbf{n} \cdot \mathbf{J}) \\ &= \frac{1}{2} \left(1 + \gamma + \frac{\alpha_1}{4} \right) \times 0.041 \text{ arcsec yr}^{-1} \\ \Omega_{\text{Geo}} &= -\frac{1}{2} (1 + 2\gamma) \mathbf{v} \times \frac{G \mathbf{m} \mathbf{n}}{r^2 c^2} \\ &= \frac{1}{3} (1 + 2\gamma) \times 6.6 \text{ arcsec yr}^{-1} \quad [8]\end{aligned}$$

where S is the spin of the gyroscope, and Ω_{FD} and Ω_{Geo} are, respectively, the precession angular velocities caused by the dragging of inertial frames (Lense–Thirring effect) and by the geodetic effect, a combination of Thomas precession and precession induced by spatial curvature; \mathbf{J} is the angular momentum of the Earth, and \mathbf{v} , \mathbf{n} , and r are, respectively, the velocity, direction, and distance of the gyroscope. The second line in each case is the corresponding value for a gyroscope in polar Earth orbit at about 650 km altitude (Gravity Probe B).

Bounds on the PPN Parameters

Four decades of high-precision experiments, ranging from the standard light-deflection and perihelion-shift tests, to LLR, planetary and satellite tracking tests of the Shapiro time delay, and geophysical and astronomical observations, have placed bounds on the PPN parameters that are consistent with GR. The current bounds are summarized in Table 1 (Will 2001).

To illustrate the dramatic progress of experimental gravity since the dawn of Einstein's theory, Figure 1 shows a history of results for $(1 + \gamma)/2$, from the 1919 solar eclipse measurements of Eddington and his colleagues (which made Einstein a celebrity), to modern-day measurements using very long baseline radio interferometry (VLBI), advanced radar tracking of spacecraft, and the astrometry satellite Hipparcos. The most recent results include a 2003 measurement of the Shapiro delay, performed by tracking the "Cassini" spacecraft on its way to Saturn, and a 2004 measurement of the bending of light via analysis of VLBI data on 541 quasars and compact radio galaxies distributed over the entire sky.

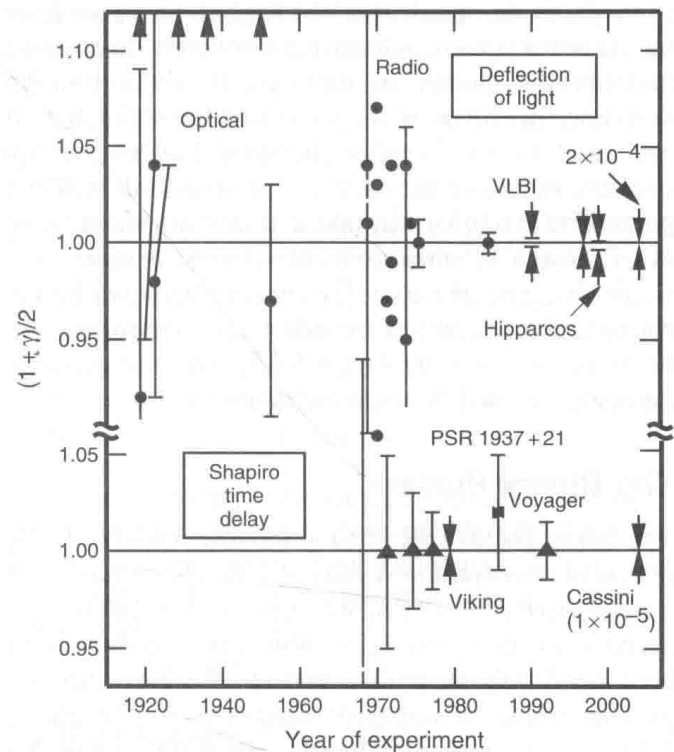


Figure 1 Measurements of the coefficient $(1 + \gamma)/2$ from observations of the deflection of light and of the Shapiro delay in propagation of radio signals near the Sun. The GR prediction is unity. "Optical" denotes measurements of stellar deflection made during solar eclipse, and "Radio" denotes interferometric measurements of radio-wave deflection. "Hipparcos" denotes the European optical astrometry satellite. Arrows denote values well off the chart from one of the 1919 eclipse expeditions and from others through 1947. Shapiro delay measurements using the Cassini spacecraft on its way to Saturn yielded tests at the 0.001% level, and light deflection measurements using VLBI have reached 0.02%.

The perihelion advance of Mercury, the first of Einstein's successes, is now known to agree with observation to a few parts in 10^3 . During the 1960s there was controversy about this test when reports of an excess solar oblateness implied an unacceptably large Newtonian contribution to the perihelion advance. However, it is now known from helioseismology, the study of short-period vibrations of the Sun, that the oblateness is of the order of a part in 10^7 , as expected from standard solar models, much too small to affect Mercury's orbit, within the observational errors.

Gravity Probe B

The NASA Relativity Mission called Gravity Probe B (GPB) recently completed its mission to measure the Lense–Thirring and geodetic precessions of gyroscopes in Earth's orbit. Launched on 20 April 2004 for a 16-month mission, it consisted of four spherical rotors coated with a thin layer of superconducting niobium, spinning at 70–100 Hz, in a spacecraft filled with liquid helium, containing a telescope continuously pointed

toward a distant guide star (IM Pegasi). Superconducting current loops encircling each rotor were designed to measure the change in direction of the rotors by detecting the change in magnetic flux through the loop generated by the London magnetic moment of the spinning superconducting film. The spacecraft was in a polar orbit at 650 km altitude. The primary science goal of GPB was a 1% measurement of the 41 marcsec yr⁻¹ frame dragging or Lense–Thirring effect caused by the rotation of the Earth; its secondary goal was to measure to six parts in 10⁵ the larger 6.6 arcsec yr⁻¹ geodetic precession caused by space curvature.

The Binary Pulsar

The binary pulsar PSR 1913 + 16, discovered in 1974, provided important new tests of GR. The pulsar, with a pulse period of 59 ms, was observed to be in orbit about an unseen companion (now generally thought to be a dead pulsar), with a period of ~ 8 h. Through precise timing of apparent variations in the pulsar “clock” caused by the Doppler effect, the important orbital parameters of the system could be measured with exquisite precision. These included nonrelativistic “Keplerian” parameters, such as the eccentricity e , and the orbital period (at a chosen epoch) P_b , as well as a set of relativistic “post-Keplerian” (PK) parameters. The first PK parameter, $\langle \dot{\omega} \rangle$, is the mean rate of advance of periastron, the analog of Mercury’s perihelion shift. The second, denoted γ' , is the effect of special relativistic time dilation and the gravitational redshift on the observed phase or arrival time of pulses, resulting from the pulsar’s orbital motion and the gravitational potential of its companion. The third, \dot{P}_b , is the rate of decrease of the orbital period; this is taken to be the result of gravitational radiation damping (apart from a small correction due to the acceleration of the system in our rotating galaxy). Two other parameters, s and r , are related to the Shapiro time delay of the pulsar signal if the orbital inclination is such that the signal passes in the vicinity of the companion; s is a direct measure of the orbital

inclination $\sin i$. According to GR, the first three PK effects depend only on e and P_b , which are known, and on the two stellar masses, which are unknown. By combining the observations of PSR 1913 + 16 (see Table 2) with the GR predictions, one obtains both a measurement of the two masses and a test of GR, since the system is overdetermined. The results are

$$m_1 = 1.4414 \pm 0.0002 M_\odot, \quad m_2 = 1.3867 \pm 0.0002 M_\odot$$

$$\dot{P}_b^{\text{GR}} / \dot{P}_b^{\text{OBS}} = 1.0013 \pm 0.0021 \quad [9]$$

Other relativistic binary pulsars may provide even more stringent tests. These include the relativistic neutron star/white dwarf binary pulsar J1141-6545, with a 0.19 day orbital period, which may ultimately lead to a very strong bound on the phenomenon of dipole gravitational radiation, predicted by many alternative theories of gravity, but not by GR; and the remarkable “double pulsar” J0737-3039, a binary system with two detected pulsars, in a 0.10 day orbit seen almost edge on and a periastron advance of 17° per year. For further discussion of binary pulsar tests, see Stairs (2003).

Gravitational-Wave Tests

The detection of gravitational radiation by either laser interferometers or resonant cryogenic bars will usher in a new era of gravitational-wave astronomy (Barish and Weiss 1999). Furthermore, it will yield new and interesting tests of GR in its radiative regime (Will 1999).

GR predicts that gravitational waves possess only two polarization modes independently of the source; they are transverse to the direction of propagation and quadrupolar in their effect on a detector. Other theories of gravity may predict up to four additional modes of polarization. A suitable array of gravitational antennas could delineate or limit the number of modes present in a given wave. If distinct evidence were found of any mode other than the two transverse quadrupolar modes of GR, the result would be disastrous for the theory.

Table 2 Parameters of the binary pulsars PSR 1913 + 16 and J0737-3039

Parameter	Symbol	Value ^a in PSR1913 + 16	Value ^a in J0737-3039
<i>Keplerian parameters</i>			
Eccentricity	e	0.6171338(4)	0.087779(5)
Orbital period	P_b (day)	0.322997448930(4)	0.102251563(1)
<i>Post-Keplerian parameters</i>			
Periastron advance	$\langle \dot{\omega} \rangle (^{\circ}\text{yr}^{-1})$	4.226595(5)	16.90(1)
Redshift/time dilation	γ' (ms)	4.2919(8)	0.382(5)
Orbital period derivative	$\dot{P}_b (10^{-12})$	-2.4184(9)	
Shapiro delay ($\sin i$)	s		0.9995(4)

^aNumbers in parentheses denote errors in last digit.

According to GR, gravitational waves propagate with the same speed, c , as light. In other theories, the speed could differ from c because of coupling of gravitation to “background” gravitational fields, or propagation of the waves into additional spatial dimensions. Another way in which the speed of gravitational waves could differ from c is if gravitation were propagated by a massive field (a massive graviton), in which case v_g would be given by, in a local inertial frame,

$$\frac{v_g^2}{c^2} = 1 - \frac{m_g^2 c^4}{E^2} \approx 1 - \frac{c^2}{f^2 \lambda_g^2} \quad [10]$$

where m_g , E , and f are the graviton rest mass, energy, and frequency, respectively, and $\lambda_g = h/m_g c$ is the graviton Compton wavelength (it is assumed that $\lambda_g \gg c/f$).

The most obvious way to measure the speed of gravitational waves is to compare the arrival times of a gravitational wave and an electromagnetic wave from the same event (e.g., a supernova). For a source at a distance of 600 million light years (a typical distance for the currently operational detectors), and a difference in times on the order of seconds, the bound on the difference $|1 - v_g/c|$ could be as small as a part in 10^{17} . It is worth noting that a 2002 report that the speed of gravity had been measured by studying light from a quasar as it propagated past Jupiter was fundamentally flawed. That particular measurement was not sensitive to the speed of gravity.

Conclusions

The past four decades have witnessed a systematic, high-precision experimental verification of Einstein's theories. Relativity has passed every test with flying colors. A central theme of future work will be to test strong-field gravity in the vicinity of black holes and

neutron stars, and to see how well GR works on cosmological scales. Gamma-ray, X-ray, microwave, infrared, neutrino, and gravitational-wave astronomy will all play a critical role in probing these largely unexplored aspects of GR.

GR is now the “standard model” of gravity. But, as in particle physics, there may be a world beyond the standard model. Quantum gravity, strings, and branes may lead to testable effects beyond Einstein's GR. Searches for such effects using laboratory experiments, particle accelerators, space instrumentation, and cosmological observations are likely to continue for some time to come.

See also: Cosmology: Mathematical Aspects; Einstein Equations: Exact Solutions; General Relativity: Overview; Geometric Flows and the Penrose Inequality; Gravitational Lensing; Gravitational Waves; Standard Model of Particle Physics.

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General Relativity: Overview

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The Principle of Equivalence

The special theory of relativity is founded on two basic principles: that the laws of physics should be independent of the uniform motion of an inertial frame of reference, and that the speed of light should have the same constant value in any such frame. In the years between 1905 and 1915, Einstein pondered deeply on what was, to him, a

profound enigma, which was the issue of why these laws retain their proper form only in the case of an inertial frame. In special relativity, as had been the case in the earlier dynamics of Galilei–Newton, the laws indeed retain their basic form only when the reference frame is unaccelerated (which includes it being nonrotating). It demonstrated a particular prescience on the part of Einstein that he should have demanded the seemingly impossible requirement that the very same dynamical laws should hold also in an accelerating (or even rotating) reference frame. The key realization came to him late in 1907, when sitting in his chair in the Bern

patent office he had the “happiest thought” in his life, namely that if a person were to fall freely in a gravitational field, then he would not notice that field at all while falling. The physical point at issue is Galileo’s early insight (itself having roots even earlier from Simon Stevin in 1586 or Ioannes Philiponos in the fifth or sixth century) that the acceleration induced by gravity is independent of the body upon which it acts. Accordingly, if two neighboring bodies are accelerated together in the same gravitational field, then the motion of one body, in the (nonrotating) reference frame of the other, will be as though there were no gravitational field at all. To put this another way, the effect of a gravitational force is just like that of an accelerating reference system, and can be eliminated by free fall. This is now known as the “principle of equivalence.”

It should be made clear that this is a particular feature of only the gravitational field. From the perspective of Newtonian dynamics, it is a consequence of the seemingly accidental fact that the concept of (passive) “mass” m that features in Newton’s law of gravitational attraction, where the attractive force due to the gravitational field of another body, of mass M , has the form

$$\frac{GmM}{r^2}$$

is the same as – or, at least, proportional to – the inertial mass m of the body which is being acted upon. Thus, the impedance to acceleration of a body and the strength of the attractive force on that body are, in the case of gravity (and only in the case of gravity), in proportion to one another, so that the acceleration of a body in a gravitational field is independent of its mass (or, indeed, of any other localized magnitude) possessed by it. (The fact that the active gravitational mass, here given by the quantity M , is also in proportion to its own passive gravitational mass – from Newton’s third law – may be regarded as a feature of the general Lagrangian/Hamiltonian framework of physics. But see Bondi (1957).) Other forces of nature do not have this property. For example, the electrostatic force on a charged body, by an electric field, acts in proportion to the electric charge on that body, whereas, the impedance to acceleration is still the inertial mass of that body, so the acceleration induced depends on the charge-to-mass ratio. Accordingly, it is the gravitational field alone which is equivalent to an acceleration.

Einstein’s fundamental idea, therefore, was to take the view that the “relativity principle” could as well be applied to accelerating reference frames as to inertial ones, where the same physical laws would apply in each, but where now the perceived

gravitational field would be different in the two frames. In accordance with this perspective, Einstein found it necessary to adopt a different viewpoint from the Newtonian one, both with regard to the notion of “gravitational force” and to the very notion of an “inertial frame.” According to the Newtonian perspective, it would be appropriate to describe the action of the Earth’s gravitational field, near some specific place on the Earth’s surface, in terms of a “Newtonian inertial frame” in which the Earth is “fixed” (here we ignore the Earth’s rotation and the Earth’s motion about the Sun), and we consider that there is a constant gravitational field of force (directed towards the Earth’s center). But the Einsteinian perspective is to regard that frame as noninertial where, instead, it would be a frame which falls freely in the Earth’s (Newtonian) gravitational field that would be regarded as a suitable “Einsteinian inertial frame.” Generally, to be inertial in Einstein’s sense, the frame would refer to free fall under gravity, so that the Newtonian field of gravitational force would appear to have disappeared – in accordance with his “happiest thought” that Einstein had had in the Bern patent office. We see that the concept of a gravitational field must also be changed in the passage from Newton’s to Einstein’s viewpoint. For in Newton’s picture we indeed have a “gravitational force” directed towards the ground with a magnitude of gm , where m is the mass of the body being acted upon and g is the “acceleration due to gravity” at the Earth’s surface, whereas in Einstein’s picture we have specifically eliminated this “gravitational force” by the choice of “Einsteinian inertial frame.”

It might at first seem puzzling that the gravitational field has appeared to have been removed altogether by this device, and it is natural to wonder how gravitational effects can have any physical role to play at all from this point of view! However, this would be to go too far, as the Newtonian gravitational field may vary from place to place – as it does, indeed, in the case of the Earth’s field, since it is directed towards the Earth’s center, which is a different spatial direction at different places on the Earth’s surface. Our considerations up to this point really refer only to a small neighborhood of a point. One might well take the view that a “frame” ought really to describe things also at widely separated places at once, and the considerations of the paragraphs above do not really take this into consideration.

The Tidal Effect

To proceed further, it will be helpful to consider an astronaut A in free fall, high above the Earth’s surface. Let us first adopt a Newtonian perspective.

We shall be concerned only with the instantaneous accelerations due to gravity in the neighborhood of A, so it will be immaterial whether we regard the astronaut as falling to the ground or – more comfortably! – in orbit about the Earth.

Let us imagine that the astronaut is initially surrounded, nearby, by a sphere of particles, with A at the centre, which are taken to be initially at rest with respect to A (see **Figure 1**). To a first approximation, all the particles will share the same acceleration as the astronaut, so they will seem to the astronaut to hover motionless all around. But now let us be a little more precise about the accelerations. Those particles which are initially located in a vertical line from A, that is, either directly below A, at B, or directly above A, at T, will have, like A, an acceleration which is in the direction AO, where O is the Earth's center. But for the bottom point B, the acceleration will be slightly greater than that at A, and for the top point T, the acceleration will be slightly less than the acceleration at A, because of the slightly differing distances from O. Thus, relative to A, both will initially accelerate away from A. With regard to particles in the sphere which are initially in a circle in the horizontal plane through A, the direction to O will now be somewhat inwards, so that the particles

at these points H_i will accelerate, relative to A, slightly inwards. Accordingly, the entire sphere of particles will begin to get distorted into a prolate spheroid (elongated ellipsoid of revolution). This is referred to as the tidal distortion, for the good reason that it is precisely the same physical effect which is responsible for the tides in the Earth's oceans, where for this illustration we are to think of the Earth's center as being at A, the Moon (or Sun) to be situated at O, and the sphere of particles to represent the surface of the water of the Earth's oceans.

It is not hard to calculate (reverting, now, to our original picture) that, as a reflection of Newton's inverse-square law of gravitational attraction, the amount of (small) outward vertical displacement from A (at B and T) will be twice the inward horizontal displacement (over the circle of points H_i); accordingly, the sphere will initially be distorted into an ellipsoid of the same volume. This depends upon there being no gravitating matter inside the sphere. The presence of such matter would contribute a volume-reducing effect in proportion to the total mass surrounded. (An extreme case illustrating this would occur if we take our sphere of particles to surround the entire Earth, where the volume-reducing effect would be manifest in the accelerations towards the ground at all points of the surrounding sphere.)

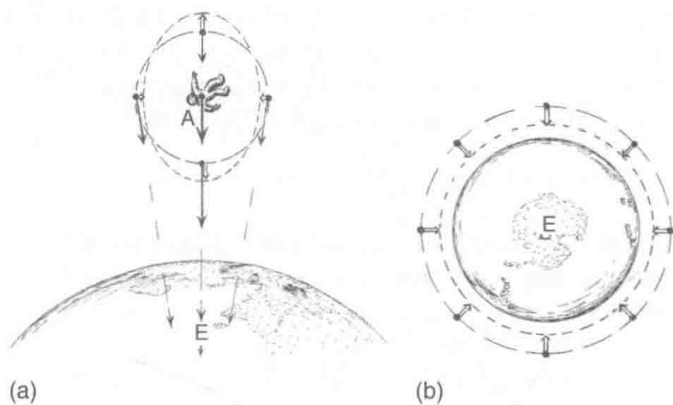


Figure 1 (a) Tidal effect. The astronaut A surrounded by a sphere of nearby particles initially at rest with respect to A. In Newtonian terms, they have an acceleration towards the Earth's center E, varying slightly in direction and magnitude (single-shafted arrows). By subtracting A's acceleration from each, we obtain the accelerations relative to A (double-shafted arrows); this relative acceleration is slightly inward for those particles displaced horizontally from A, but slightly outward for those displaced vertically from A. Accordingly, the sphere becomes distorted into a (prolate) ellipsoid of revolution, with symmetry axis in the direction AE. The initial distortion preserves volume. (b) Now move A to the Earth's center E and the sphere of particles to surround E just above the atmosphere. The acceleration (relative to $A=E$) is inward all around the sphere, with an initial volume reduction acceleration $4\pi GM$, where M is the total mass surrounded. Reproduced with permission from Penrose R (2004) *The Road to Reality: A Complete Guide to the Laws of the Universe*. London: Jonathan Cape.

Gravity as Curved Spacetime

It is appropriate to take a spacetime view of these phenomena (**Figure 2**). The distortions that we have been considering are, in fact, direct manifestations

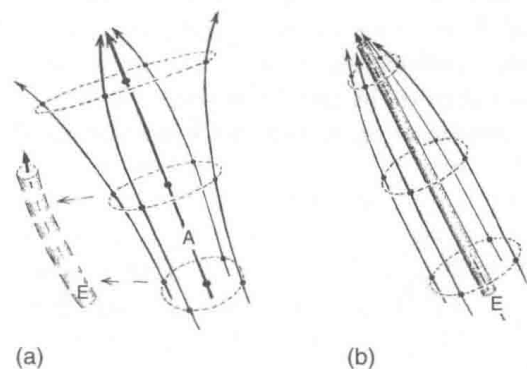


Figure 2 Spacetime versions of **Figure 1** in terms of the relative distortion of neighboring geodesics. (a) Geodesic deviation in empty space (basically Weyl curvature) as seen in the world lines of A and surrounding particles (one spatial dimension suppressed), as might be induced from the gravitational field of a nearby body E. (b) The corresponding inward acceleration (basically Ricci curvature) due to the mass density within the bundle of geodesics. Reproduced with permission from Penrose R (2004) *The Road to Reality: A Complete Guide to the Laws of the Universe*. London: Jonathan Cape.

of spacetime curvature, according to Einstein's viewpoint. We are to think of the world line of a particle, falling freely under gravity (Einsteinian inertial motion), as described as some kind of geodesic in spacetime. We shall be coming to this more completely shortly, but for the moment it will be helpful to picture the behavior of geodesics within an ordinary curved 2-surface S (Figure 3). If S has positive (Gaussian) curvature, then there will be a tendency for geodesics on S to bend towards each other, so that a pair of infinitesimally separated geodesics which are initially parallel will begin to get closer together as we move along them; if S has negative (Gaussian) curvature, then there will be a corresponding tendency for geodesics on S to bend away from each other. This is what happens in two dimensions, where the intrinsic curvature at a point is given by a single number. However, we are now concerned with a four-dimensional space, where the notion of curvature requires many more components. We see in Figure 2 that we are indeed to expect mixtures of convergence and divergence of geodesics, which suggests that there are both positive and negative curvature components involved, the positive curvature being in the horizontally displaced directions from A and the negative curvature in the vertically displaced directions. In a curved space of dimension 4, as is the case for a curved spacetime, we can expect 20 independent components of curvature at each point altogether. In the present situation, the others would be called into play when differing velocities of A are considered.

Let us see how we are to accommodate the above considerations within the standard framework of differential geometry. So far, we have not really deviated from Newtonian theory, even though we have been considering "geodesics" in a four-dimensional spacetime. In fact, it is perfectly legitimate to view Newtonian theory in this way (see Newtonian

Limit of General Relativity), although the 4-geometry description is somewhat more complicated than one might wish. This is due to the fact that the infinite speed at which gravitation is taken to act in Newtonian theory demands that the "metric" of Newtonian spacetime is degenerate. (In effect, one would have a degenerate "dual metric" G^{ab} , of matrix rank 3, which plays a role in defining spatial displacements and a very degenerate "metric" G_{ab} , of matrix rank 1, which defines temporal differences, where $G^{ab}G_{bc}=0$; see Newtonian Limit of General Relativity.) Accordingly, there is no unique notion of "geodesic" defined by the metric in Newtonian theory.

It is striking that although the insights provided by the principle of equivalence are to some considerable extent independent of special relativity (since we see from the paragraphs prior to the preceding one that a curved-spacetime-geometry view of gravity is natural in the light of the equivalence principle alone), it is the nondegenerate metric g_{ab} , (and its inverse g^{ab}) that special relativity gives us locally, which leads to an elegant spacetime theory of gravity. Although the metric g_{ab} is Lorentzian (with preferred choice of signature $+- --$ here) rather than positive definite, so that the spacetime is not strictly a Riemannian one, the change of signature makes little difference to the local formalism. In particular, the fact that the metric defines a unique (torsion-free) connection preserving it is unaffected by the signature. This connection is the one defined by Christoffel's symbols

$$\Gamma_{ac}{}^b = \frac{1}{2}g^{db}(\partial_c g_{da} + \partial_a g_{cd} - \partial_d g_{ca})$$

where ∂_a stands for coordinate derivative $\partial/\partial x^a$, so that the covariant derivative of a vector V^a is given by

$$\nabla_a V^b = \partial_a V^b + V^c \Gamma_{ac}{}^b$$

(Here the standard "physicist's conventions" are being used, whereby notation such as " g_{ab} " and " V^a " can be used interchangeably either for the sets of components of the metric tensor g and the vector V , respectively, or alternatively for the entire geometrical metric tensor g or vector V , in each case; moreover, the summation convention is being assumed, or this can alternatively be understood in terms of abstract indices. (For the abstract-index notation for tensors, see Penrose and Rindler (1984), especially Chapters 2 and 4. Sign and index-ordering conventions used here follow those given in that book. Many other authors use conventions which differ from these in various, usually minor respects.))

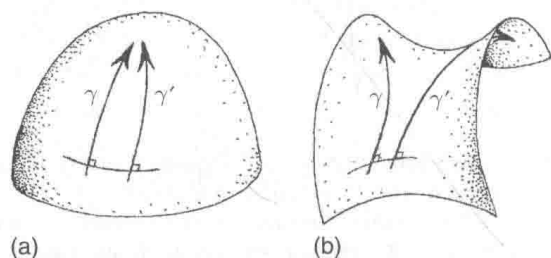


Figure 3 Geodesic deviation when M is a 2-surface (a) of positive (Gaussian) curvature, when the geodesics γ, γ'' bend towards each other, and (b) of negative curvature, when they bend apart. Reproduced with permission from Penrose R (2004) *The Road to Reality: A Complete Guide to the Laws of the Universe*. London: Jonathan Cape.

Physical Interpretation of the Metric

Some words of clarification are needed, as to the meaning of the metric tensor g_{ab} in relativity theory. In the early discussions by Einstein and others, the spacetime metric tended to be interpreted in terms of little “rulers” placed on a curved manifold. Although this is natural in the Riemannian (positive-definite) case, it is not quite so appropriate for the Lorentzian geometry of spacetime manifolds. An ordinary physical ruler has a spacetime description as a timelike strip, and it does not naturally express the spatial separation between two spacelike-separated events. In order for a ruler to measure such a spacelike separation, it would be necessary for the two events to be simultaneous in the ruler’s rest frame, and for this to be assured, some further mechanism would be needed, such as Einstein’s procedure for ensuring simultaneity by the use of light signals from the two events to be received simultaneously at their midpoint on the ruler. Clearly this complicates the issue, and it turns out to be much preferable to concentrate on temporal displacements rather than spatial ones.

The idea that spacetime geometry should really be regarded as “chronometry,” in this way, has been stressed by a number of distinguished expositors of relativity theory, most notably John L Synge (1956, 1960) and Hermann Bondi (1961, 1964, 1967). Where needed, spatial displacements can then be defined by the use of temporal ones together with light signals. This has the additional advantage that in modern technology, the measurement of (proper) time far surpasses that of distance in accuracy, to the extent that the meter is now defined simply by the requirement that there are exactly 299792458 of them in a light-second! The proper time interval between two nearby events is, indeed, measured by a clock which encounters both events, moving inertially between the two, and very precise atomic and nuclear clocks are now a common feature of current technology. The physical role of the metric g_{ab} is most clearly seen in the formula

$$\tau = \int_p^q (g_{ab} dx^a dx^b)$$

which measures the (proper) time interval τ between an event p and a later event q on its world line, the integral being taken along this curve, and where now that curve need not be a geodesic, so that accelerating (noninertial) motion of the clock is allowed. The metric (with choice of signature $+- - -$ so that it is the timelike displacements that are directly provided as real numbers) is very precisely specified by this physical requirement, and this tells us that the

pseudo-Riemannian (Lorentzian) structure of spacetime is far from being an arbitrary construction, but is given to us by Nature with enormous precision. (Some theorists prefer to use the alternative spacetime signature $-+++$, because this more directly relates to familiar Newtonian concepts, these being normally described in spatial terms. The difference is essentially just a notational one, however. It may be remarked that the 2-spinor formalism (see Spinors and Spin Coefficients) fits in much more readily with the $+- - -$ signature being used here.) It may be noted, also that this time measure is ultimately fixed by quantum principles and the masses of the elementary ingredients involved (e.g., particle masses) via the Einstein and Planck relations $E = mc^2$ and $E = h\nu$, so that there is a natural frequency associated with a given mass, via $\nu = mc^2/h$ (c being the speed of light and h being Planck’s constant).

Riemann Curvature and Geodesic Deviation

The unique torsion-free (Christoffel–Levi-Civita) connection ∇_a is, via this physically determined metric, also fixed accordingly by these physical considerations, as is the notion of a geodesic, and therefore so also is the curvature. The 20-independent-component Riemann curvature tensor R_{abcd} may be defined by

$$(\nabla_a \nabla_b - \nabla_b \nabla_a) V^d = R_{abc}{}^d V^c$$

with normal index-raising/lowering conventions, so that $R_{abcd} = R_{abc}{}^e g_{ed}$, etc., and we have the standard classical formula

$$R_{abc}{}^d = \partial_a \Gamma_{cb}{}^d - \partial_b \Gamma_{ca}{}^d + \Gamma_{cb}{}^e \Gamma_{ea}{}^d - \Gamma_{ca}{}^e \Gamma_{eb}{}^d$$

The symmetries $R_{abcd} = R_{cdab} = -R_{bacd}$, $R_{abcd} + R_{bcad} + R_{cabd} = 0$ reduce the number of independent components of R_{abcd} to 20 (from a potential $4^4 = 64$). Of these, 10 are locally fixed by the kind of physical requirement indicated above, that in order to express something that agrees closely with Newton’s inverse-square law we require that there should be a net inward curving of free world lines (the timelike geodesics that represent local inertial motions, or “free fall” under gravity). Let us see how this requirement is satisfied in Einstein’s general relativity.

What we find, from Newton’s theory, is that a system of test particles which, at some initial time constitutes a closed 2-surface at rest surrounding some gravitating matter, will begin to accelerate in such a way that the volume surrounded is initially reduced in proportion to the total mass surrounded.

This volume reduction is a direct consequence of Poisson's equation $\nabla^2\Phi = -4\pi\rho$ (Φ being the gravitational potential and ρ the mass density) and of Newton's second law, which tell us that the second time derivative of the free-fall volume of our initially stationary closed surface of test particles is indeed $-4\pi GM$, where M is the total gravitating mass surrounded (and G is Newton's constant, as above). In Einstein's theory, we can basically carry this over to our four-dimensional Lorentzian spacetime. We do, however, find that such a general statement as this does not exactly hold. Instead of referring to 3-volumes of any size, we must restrict attention to infinitesimal volumes.

The basic mathematical tool is the equation of "geodesic deviation," namely the "Jacobi equation":

$$D^2 u^d = R_{abc}{}^d t^a u^b t^c$$

where D describes "propagation derivative"

$$D = t^a \nabla_a$$

along a timelike geodesic γ , where t^a is a unit timelike tangent vector to γ (so $t_a t^a = g_{ab} t^a t^b = 1$) which is (consequently) parallel-propagated along γ ,

$$D t^a = 0$$

(When acting on a scalar quantity defined along γ , we can read " D " as " $d/d\tau$," where τ measures proper time along γ .) The vector u^a is what is called a connecting vector between the geodesic γ and some "neighboring geodesic" γ' . We think of the vector u^a as "connecting" a point p on γ to some neighboring point p' on γ' , where it is usual to take u^a to be orthogonal to t^a (i.e., $u_a t^a = 0$). The derivative Du^a measures the rate of change of u^a , as p and p' move together into the future along γ . Mathematically, we express this as the vanishing of the Lie derivative of u^a with respect to t^a (with t_a extended to a unit vector field which is tangent both to γ and to γ'). By taking three independent vectors u^a at p , we can form a spatial 3-volume element W and investigate how this propagates along γ . We find

$$D^2 W = W R_{ab} t^a t^b$$

where the Ricci tensor $R_{ab}(=R_{ba})$ is here defined by

$$R_{ab} = R_{acb}{}^c$$

The Einstein Field Equations

In view of what has been said above, with regard to the way that the acceleration of volume behaves in Newtonian theory, it would be natural to "identify" $R_{ab} t^a t^b$ with $(-4\pi G \times)$ the (active gravitational) mass density, with respect to the time

direction t^a . In (special) relativity theory we expect to identify mass density with $c^{-2} \times$ energy density (by $E=mc^2$) and to take energy density as just one component (the time-time component) of a symmetric tensor T_{ab} , called the "energy tensor," and for simplicity we now take $c=1$. The tensor quantity T_{ab} is to incorporate the contributions to the local mass/energy density of all particles and fields other than gravity itself. Since we would require this to work for all choices of time-direction t^a , it would be natural, accordingly, to make the identification

$$R_{ab} = -4\pi G T_{ab}$$

Indeed, this was Einstein's initial choice for a gravitational field equation. However, this will actually not do, as Einstein later realized. The trouble comes from the Bianchi identity

$$\nabla_a R_{bcde} + \nabla_b R_{cade} + \nabla_c R_{abde} = 0$$

from which we deduce

$$\nabla^a (R_{ab} - \frac{1}{2} R g_{ab}) = 0$$

where

$$R = R_a{}^a$$

This causes trouble in connection with the standard requirement on the energy tensor, that it satisfy the local "conservation law"

$$\nabla^a T_{ab} = 0$$

The latter equation is an essential requirement in special relativity, since it expresses the conservation of energy and momentum for fields in flat spacetime. In standard Minkowski coordinates, each of $T_{a0}, T_{a1}, T_{a2}, T_{a3}$ satisfies an equation just like the $\nabla^a J_a = 0$ of the charge-current vector J_a of Maxwell's theory of electromagnetism, with now $\nabla_a = \partial_a = \partial/\partial x^a$, which expresses global conservation of charge. Similarly to the way that J_a encapsulates density and flux of electric charge, T_{a0} encapsulates density and flux of energy, and T_{a1}, T_{a2}, T_{a3} encapsulate the same for the three components of momentum. So the equation $\nabla^a T_{ab} = 0$ is essential in special relativity, for similarly expressing global conservation of energy and momentum. We find (referring to a local inertial frame) that, when we pass to general relativity, this equation should still hold, with ∇_a now standing for covariant derivative. But the initially proposed field equation $R_{ab} = -4\pi G T_{ab}$ would now give us $\nabla^a R_{ab} = 0$, which combined with the geometrically necessary $\nabla^a (R_{ab} - (\frac{1}{2}) R g_{ab}) = 0$, tells us that R is constant. In turn this implies the physically unacceptable requirement that $T = T_a{}^a$ is constant (since we have $R = -4\pi G T$).

Einstein eventually became convinced (by 1915) of the modified field equations

$$R_{ab} - \frac{1}{2}Rg_{ab} = -8\pi GT_{ab}$$

(the “8” rather than “4” being now needed to fit in with the Newtonian limit) and it is these that are now commonly referred to as “Einstein’s field equations.” (Some authors prefer to use the singular form “field equation,” especially if the formula is to be read as an abstract-index expression rather than a family of component equations, since the tensors involved are really single entities.) It may be noted that the formula can be rewritten as

$$R_{ab} = -8\pi G(T_{ab} - \frac{1}{2}Tg_{ab})$$

from which we deduce that in Einstein’s theory the source of gravity is not simply the mass (or equivalently energy) density, but there is an additional contribution from the pressure (momentum flux, i.e., space-space components of T_{ab}). This can have significant implications for the instability of very large and massive stars in highly relativistic regimes, where increases in pressure can, paradoxically, actually increase the tendency for a star to collapse, owing to its contribution to the attractive effect of its gravity.

In 1917, Einstein put forward a slight modification of his field equations – basically the only modification that can be made without fundamentally changing the foundations of his theory – by introducing the very tiny cosmological constant Λ . The modified equations are

$$R_{ab} - \frac{1}{2}Rg_{ab} + \Lambda g_{ab} = -8\pi GT_{ab}$$

and the source of gravity, or active gravitational mass is now

$$\rho + P_1 + P_2 + P_3 - \frac{\Lambda}{4\pi G}$$

where (with respect to a local Lorentzian orthonormal frame, units being chosen so that $c=1$) $\rho = T_{00}$ is the mass/energy density and $P_1 = T_{11}$, $P_2 = T_{22}$, $P_3 = T_{33}$ are the principal pressures. The Λ -term, for positive Λ , provides a repulsive contribution to the gravitational effect, but it is extremely tiny (and totally ignorable) on all ordinary scales, beginning to show itself only at the most vast of observed cosmological distances (since the effect of Λ adds up relentlessly at larger and larger distances). Einstein originally introduced the term in order to have the possibility of a static universe, where the attractive gravitational effect of the totality of ordinary matter would be balanced, overall, by Λ . But the discovery of the expansion of the universe (by Hubble and others) led Einstein to abandon the cosmological term. However, since 1998 (initially

from the supernova observations of Brian Schmidt and Robert Kirshner, and Saul Perlmutter, *see* Perlmutter *et al.* (1998)), cosmological evidence has mounted in favor of the presence of a very small positive Λ -term, which has resulted in the expansion of the universe beginning to accelerate. While the presence of Einstein’s constant Λ -term is consistent with observations, and remains the simplest explanation of this observed acceleration, many cosmologists prefer to allow for what would amount to a “varying Λ ,” and refer to it as “dark energy.”

Energy Conservation and Related Matters

One of the features of Einstein’s general relativity theory that had been deeply puzzling to a good many of Einstein’s contemporaries, and which may be said to be still not fully resolved, even today, is “energy conservation,” in the presence of a dynamical gravitational field. We have noted that the energy tensor T_{ab} is to incorporate the contributions of all particles and fields other than gravity. But what about gravity itself? There are many physical situations in which energy can be transferred back and forth from gravitational systems to nongravitational ones (most strikingly in the example of the emission of gravitational waves; *see* Gravitational Waves). The conservation of energy would make no sense without an understanding of how energy can be stored in a gravitational field. At first sight we seem to see no role for a gravitational contribution to energy in Einstein’s theory, since the conservation law $\nabla^a T_{ab} = 0$ seems to be a self-contained expression of energy conservation with no direct contribution from the gravitational field in the tensor T_{ab} . However, this is illusory, since the formulation of a global conservation law from the local covariant expression $\nabla^a T_{ab} = 0$ does not work in curved spacetime (basically because, unlike the charge-current quantity J_a of Maxwell’s electrodynamical theory, the extra index on T_{ab} prevents it from being regarded as a 1-form). We may take the view that the energy of gravitation enters nonlocally into the equation, so that the failure of T_{ab} to provide a global conservation law on its own is an expression of the gravitational contributions of energy not being taken into account. This is no doubt a correct attitude to take, but it is a difficult one to express comprehensively in a mathematical form. Einstein himself provided a partial understanding, but at the expense of introducing concepts known as “pseudotensors” whose meaning was too tied up with arbitrary choices of coordinate systems to provide an overall picture. In modern approaches, the most clear-cut results come from the study of asymptotically flat or asymptotically de Sitter spacetimes (de Sitter space being the empty universe which takes over the role of Minkowski space when

there is a positive cosmological constant Λ ; see Cosmology: Mathematical Aspects).

The important role of the “Weyl conformal tensor”

$$C_{abcd} = R_{abcd} - \frac{1}{2}(R_{ac}g_{bd} - R_{bc}g_{ad} + R_{bd}g_{ac} - R_{ad}g_{bc}) + \frac{1}{6}R(g_{ac}g_{bd} - g_{bc}g_{ad})$$

should also be pointed out. This tensor retains all the symmetries of the full Riemann tensor, but has the Ricci tensor contribution removed, so that all its contractions vanish, as is exemplified by

$$C_{abc}{}^a = 0$$

It describes the conformal part of the curvature, that is, that part that survives under conformal rescalings of the metric;

$$g_{ab} \mapsto \Omega^2 g_{ab}$$

where Ω is a smooth (positive) function of position. The tensor $C_{abc}{}^d$ is itself invariant under these conformal rescalings. This has importance in the asymptotic analysis of gravitational fields (see Asymptotic Structure and Conformal Infinity). We may take the view that C_{abcd} describes the degrees of freedom in the free gravitational field, whereas R_{ab} contains the information of the sources of gravity. This is analogous to the Maxwell tensor F_{ab} describing the degrees of freedom in the free electromagnetic field, whereas J_a contains the information of the sources of electromagnetism.

From the observational point of view, general relativity stands in excellent shape, with full agreement with all known relevant data, starting with the anomalous perihelion advance of the planet Mercury observed by LeVerrier in the mid-nineteenth century, through clock-slowness, light-bending (lensing) and time-delay effects, and the necessary corrections to GPS positioning systems, to the precise orbiting of double neutron-star systems, with energy loss due to the emission of gravitational waves. The effects of gravitational lensing now play vital roles in modern cosmology.

To get some idea of the precision in Einstein's theory, we may take note of the fact that the double neutron-star system PSR 1913+16 has been observed for some 30 years, and the agreement between observation and theory overall is to about one part in 10^{14} .

See also: Asymptotic Structure and Conformal Infinity; Canonical General Relativity; Computational Methods in General Relativity: the Theory; Cosmology: Mathematical Aspects; Einstein Equations: Exact Solutions; Einstein Equations: Initial Value Formulation; Einstein–Cartan Theory; Einstein's Equations with Matter; General Relativity: Experimental Tests; Geometric Flows and the Penrose Inequality; Gravitational Lensing; Gravitational Waves; Hamiltonian Reduction of Einstein's Equations; Lorentzian Geometry; Newtonian Limit of General Relativity; Noncommutative geometry and the Standard Model; Spacetime Topology, Causal Structure and Singularities; Spinors and Spin Coefficients; Symmetries and Conservation Laws; Twistor Theory: Some Applications [in Integrable Systems, Complex Geometry and String Theory].

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Generic Properties of Dynamical Systems

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Introduction

The state of a concrete system (from physics, chemistry, ecology, or other sciences) is described using (finitely many, say n) observable quantities (e.g., positions and velocities for mechanical systems, population densities for ecological systems, etc.). Hence, the state of a system may be

represented as a point x in a geometrical space \mathbb{R}^n . In many cases, the quantities describing the state are related, so that the phase space (space of all possible states) is a submanifold $M \subset \mathbb{R}^n$. The time evolution of the system is represented by a curve $x_t, t \in \mathbb{R}$ drawn on the phase space M , or by a sequence $x_n \in M, n \in \mathbb{Z}$, if we consider discrete time (i.e., every day at the same time, or every January 1st).

Believing in determinism, and if the system is isolated from external influences, the state x_0 of the system at the present time determines its evolution. For continuous-time systems, the infinitesimal

evolution is given by a differential equation or vector field $dx/dt = X(x)$; the vector $X(x)$ represents velocity and direction of the evolution. For a discrete-time system, the evolution rule is a function $F: M \rightarrow M$; if x is the state at time t , then $F(x)$ is the state at the time $t + 1$. The evolution of the system, starting at the initial data x_0 , is described by the orbit of x_0 , that is, the sequence $\{(x_n)_{n \in \mathbb{Z}} \mid x_{n+1} = F(x_n)\}$ (discrete time) or the maximal solution x_t of the differential equation $dx/dt = X(x)$ (continuous time).

General problem *Knowing the initial data and the infinitesimal evolution rule, what can we tell about the long-time evolution of the system?*

The dynamics of a dynamical system (differential equation or function) is the behavior of the orbits, when the time tends to infinity. The aim of “dynamical systems” is to produce a general procedure for describing the dynamics of any system. For example, Conley’s theory presented in the next section organizes the global dynamics of a general system using regions concentrating the orbit accumulation and recurrence and splits these regions in elementary pieces: the chain recurrence classes.

We focus our study on C^r -diffeomorphisms F (i.e., F and F^{-1} are r times continuously derivable) on a compact smooth manifold M (most of the notions and results presented here also hold for vector fields). Even for very regular systems (F algebraic) of a low-dimensional space ($\dim(M) = 2$), the dynamics may be chaotic and very unstable: one cannot hope for a precise description of all systems. Furthermore, neither the initial data of a concrete system nor the infinitesimal-evolution rule are known exactly: fragile properties describe the evolution of the theoretical model, and not of the real system. For these reasons, we are mostly interested in properties that are persistent, in some sense, by small perturbations of the dynamical system. The notion of small perturbations of the system requires a topology on the space $\text{Diff}^r(M)$ of C^r -diffeomorphisms: two diffeomorphisms are close for the C^r -topology if all their partial derivatives of order $\leq r$ are close at each point of M . Endowed with this topology, $\text{Diff}^r(M)$ is a complete metric space.

The open and dense subsets of $\text{Diff}^r(M)$ provide the natural topological notion of “almost all” F . Genericity is a weaker notion: by Baire’s theorem, if $\mathcal{O}_i, i \in \mathbb{N}$, are dense and open subsets, the intersection $\bigcap_{i \in \mathbb{N}} \mathcal{O}_i$ is a dense subset. A subset is called residual if it contains such a countable intersection of dense open subsets. A property \mathcal{P} is generic if it is verified on a residual subset. By a practical abuse of language, one says:

“ C^r -generic diffeomorphisms verify \mathcal{P} ”

A countable intersection of residual sets is a residual set. Hence, if $\{\mathcal{P}_i\}, i \in \mathbb{N}$, is a countable family of

generic properties, generic diffeomorphisms verify simultaneously all the properties \mathcal{P}_i .

A property \mathcal{P} is C^r -robust if the set of diffeomorphisms verifying \mathcal{P} is open in $\text{Diff}^r(M)$. A property \mathcal{P} is locally generic if there is an (nonempty) open set \mathcal{O} on which it is generic, that is, there is residual set \mathcal{R} such that \mathcal{P} is verified on $\mathcal{R} \cap \mathcal{O}$.

The properties of generic dynamical systems depend mostly on the dimension of the manifold M and of the C^r -topology considered, $r \in \mathbb{N} \cup \{+\infty\}$ (an important problem is that C^r -generic diffeomorphisms are not C^{r+1}):

- On very low dimensional spaces (diffeomorphisms of the circle and vector fields on compact surfaces) the dynamics of generic systems (indeed in a open and dense subset of systems) is very simple (called Morse–Smale) and well understood; see the subsection “Generic properties of the low-dimensional systems.”
- In higher dimensions, for C^r -topology, $r > 1$, one has generic and locally generic properties related to the periodic orbits, like the Kupka–Smale property (see the subsection “Kupka–Smale theorem”) and the Newhouse phenomenon (see the subsection “Local C^2 -genericity of wild behavior for surface diffeomorphisms”). However, we still do not know if the dynamics of C^r -generic diffeomorphisms is well approached by their periodic orbits, so that one is still far from a global understanding of C^r -generic dynamics.
- For the C^1 -topology, perturbation lemmas show that the global dynamics is very well approximated by periodic orbits (see the section “ C^1 -generic systems: global dynamics and periodic orbits”). One then divides generic systems in “tame” systems, with a global dynamics analogous to hyperbolic dynamics, and “wild” systems, which present infinitely many dynamically independent regions. The notion of dominated splitting (see the section “Hyperbolic properties of C^1 -generic diffeomorphisms”) seems to play an important role in this division.

Results on General Systems

Notions of Recurrence

Some regions of M are considered as the heart of the dynamics:

- $\text{Per}(F)$ denotes the set of periodic points $x \in M$ of F , that is, $F^n(x) = x$ for some $n > 0$.
- A point x is recurrent if its orbit comes back arbitrarily close to x , infinitely many times. $\text{Rec}(F)$ denotes the set of recurrent points.
- The limit set $\text{Lim}(F)$ is the union of all the accumulation points of all the orbits of F .

- A point x is “wandering” if it admits a neighborhood $U_x \subset M$ disjoint from all its iterates $F^n(U_x)$, $n > 0$. The nonwandering set $\Omega(F)$ is the set of the nonwandering points.
- $\mathcal{R}(F)$ is the set of chain recurrent points, that is, points $x \in M$ which look like periodic points if we allow small mistakes at each iteration: for any $\varepsilon > 0$, there is a sequence $x = x_0, x_1, \dots, x_k = x$ where $d(f(x_i), x_{i+1}) < \varepsilon$ (such a sequence is an ε -pseudo-orbit).

A periodic point is recurrent, a recurrent point is a limit point, a limit point is nonwandering, and a nonwandering point is chain recurrent:

$$\text{Per}(F) \subset \text{Rec}(F) \subset \text{Lim}(F) \subset \Omega(F) \subset \mathcal{R}(F)$$

All these sets are invariant under F , and $\Omega(F)$ and $\mathcal{R}(F)$ are compact subsets of M . There are diffeomorphisms F for which the closures of these sets are distinct:

- A rotation $x \mapsto x + \alpha$ with irrational angle $\alpha \in \mathbb{R} \setminus \mathbb{Q}$ on the circle $S^1 = \mathbb{R}/\mathbb{Z}$ has no periodic points but every point is recurrent.
- The map $x \mapsto x + (1/4\pi)(1 + \cos(2\pi x))$ induces on the circle S^1 a diffeomorphism F having a unique fixed point at $x = 1/2$; one verifies that $\Omega(F) = \{1/2\}$ and $\mathcal{R}(F)$ is the whole circle S^1 .

An invariant compact set $K \subset M$ is transitive if there is $x \in K$ whose forward orbit is dense in K . Generic points $x \in K$ have their forward and backward orbits dense in K : in this sense, transitive sets are dynamically indecomposable.

Conley's Theory: Pairs Attractor/Repeller and Chain Recurrence Classes

A trapping region $U \subset M$ is a compact set whose image $F(U)$ is contained in the interior of U . By definition, the intersection $A = \bigcap_{n \geq 0} F^n(U)$ is an attractor of F : any orbit in U “goes to A .” Denote by V the complement of the interior of U : it is a trapping region for F^{-1} and the intersection $R = \bigcap_{n \geq 0} F^{-n}(V)$ is a repeller. Each orbit either is contained in $A \cup R$, or “goes from the repeller to the attractor.” More precisely, there is a smooth function $\psi: M \rightarrow [0, 1]$ (called Lyapunov function) equal to 1 on R and 0 on A , and strictly decreasing on the other orbits:

$$\psi(F(x)) < \psi(x) \quad \text{for } x \notin A \cup R$$

So, the chain recurrent set is contained in $A \cup R$. Any compact set contained in U and containing the interior of $F(U)$ is a trapping region inducing the same attractor and repeller pair (A, R) ; hence, the set of attractor/repeller pairs is countable. We denote by (A_i, R_i, ψ_i) , $i \in \mathbb{N}$, the family of these pairs endowed

with an associated Lyapunov function. Conley (1978) proved that

$$\mathcal{R}(F) = \bigcap_{i \in \mathbb{N}} (A_i \cup R_i)$$

This induces a natural partition of $\mathcal{R}(F)$ in equivalence classes: $x \sim y$ if $x \in A_i \Leftrightarrow y \in A_i$. Conley proved that $x \sim y$ iff, for any $\varepsilon > 0$, there are ε -pseudo orbits from x to y and vice versa. The equivalence classes for \sim are called chain recurrence classes.

Now, considering an average of the Lyapunov functions ψ_i , one gets the following result: there is a continuous function $\varphi: M \rightarrow \mathbb{R}$ with the following properties:

- $\varphi(F(x)) \leq \varphi(x)$ for every $x \in M$, (i.e., φ is a Lyapunov function);
- $\varphi(F(x)) = \varphi(x) \Leftrightarrow x \in \mathcal{R}(F)$;
- for $x, y \in \mathcal{R}(F)$, $\varphi(x) = \varphi(y) \Leftrightarrow x \sim y$; and
- the image $\varphi(\mathcal{R}(F))$ is a compact subset of \mathbb{R} with empty interior.

This result is called the “fundamental theorem of dynamical systems” by several authors (see Robinson (1999)).

Any orbit is φ -decreasing from a chain recurrence class to another chain recurrence class (the global dynamics of F looks like the dynamics of the gradient flow of a function ϕ , the chain recurrence classes supplying the singularities of ϕ). However, this description of the dynamics may be very rough: if F preserves the volume, Poincaré's recurrence theorem implies that $\Omega(F) = \mathcal{R}(F) = M$; the whole M is the unique chain recurrence class and the function φ of Conley's theorem is constant.

Conley's theory provides a general procedure for describing the global topological dynamics of a system: one has to characterize the chain recurrence classes, the dynamics in restriction to each class, the stable set of each class (i.e., the set of points whose positive orbits goes to the class), and the relative positions of these stable sets.

Hyperbolicity

Smale's hyperbolic theory is the first attempt to give a global vision of almost all dynamical systems. In this section we give a very quick overview of this theory. For further details, see Hyperbolic Dynamical Systems.

Hyperbolic Periodic Orbits

A fixed point x of F is hyperbolic if the derivative $DF(x)$ has no (neither real nor complex) eigenvalue with modulus equal to 1. The tangent space at x

splits as $T_x M = E^s \oplus E^u$, where E^s and E^u are the $DF(x)$ -invariant spaces corresponding to the eigenvalues of moduli < 1 and > 1 , respectively. There are C^r -injectively immersed F -invariant submanifolds $W^s(x)$ and $W^u(x)$ tangent at x to E^s and E^u ; the stable manifold $W^s(x)$ is the set of points y whose forward orbit goes to x . The implicit-function theorem implies that a hyperbolic fixed point x varies (locally) continuously with F ; (compact parts of) the stable and unstable manifolds vary continuously for the C^r -topology when F varies with the C^r -topology.

A periodic point x of period n is hyperbolic if it is a hyperbolic fixed point of F^n and its invariant manifolds are the corresponding invariant manifolds for F^n . The stable and unstable manifold of the orbit of x , $W_{\text{orb}}^s(x)$ and $W_{\text{orb}}^u(x)$, are the unions of the invariant manifolds of the points in the orbit.

Homoclinic Classes

Distinct stable manifolds are always disjoint; however, stable and unstable manifolds may intersect. At the end of the nineteenth century, Poincaré noted that the existence of transverse homoclinic orbits, that is, transverse intersection of $W_{\text{orb}}^s(x)$ with $W_{\text{orb}}^u(x)$ (other than the orbit of x), implies a very rich dynamical behavior: indeed, Birkhoff proved that any transverse homoclinic point is accumulated by a sequence of periodic orbits (see Figure 1). The homoclinic class $H(x)$ of a periodic orbit is the closure of the transverse homoclinic point associated to x :

$$H(p) = \overline{W_{\text{orb}}^s(x) \cap W_{\text{orb}}^u(x)}$$

There is an equivalent definition of the homoclinic class of x : we say that two hyperbolic periodic points x and y are homoclinically related if $W_{\text{orb}}^s(x)$ and $W_{\text{orb}}^u(x)$ intersect transversally $W_{\text{orb}}^u(y)$ and $W_{\text{orb}}^s(y)$, respectively; this defines an equivalence relation in $\text{Per}_{\text{hyp}}(F)$ and the homoclinic classes are the closure of the equivalence classes.

The homoclinic classes are transitive invariant compact sets canonically associated to the periodic

orbits. However, for general systems, homoclinic classes are not necessarily disjoint.

For more details, see Homoclinic Phenomena.

Smale's Hyperbolic Theory

A diffeomorphism F is *Morse–Smale* if $\Omega(F) = \text{Per}(F)$ is finite and hyperbolic, and if $W^s(x)$ is transverse to $W^u(y)$ for any $x, y \in \text{Per}(F)$. Morse–Smale diffeomorphisms have a very simple dynamics, similar to the one of the gradient flow of a Morse function; apart from periodic points and invariant manifolds of periodic saddles, each orbit goes from a source to a sink (hyperbolic periodic repellers and attractors). Furthermore, Morse–Smale diffeomorphisms are C^1 -structurally stable, that is, any diffeomorphism C^1 -close to F is conjugated to F by a homeomorphism: the topological dynamics of F remains unchanged by small C^1 -perturbation. Morse–Smale vector fields were known (Andronov and Pontryagin, 1937) to characterize the structural stability of vector fields on the sphere S^2 . However, a diffeomorphism having transverse homoclinic intersections is robustly not Morse–Smale, so that Morse–Smale diffeomorphisms are not C^r -dense, on any compact manifold of dimension ≥ 2 . In the early 1960s, Smale generalized the notion of hyperbolicity for nonperiodic sets in order to get a model for homoclinic orbits. The goal of the theory was to cover a whole dense open set of all dynamical systems.

An invariant compact set K is hyperbolic if the tangent space $TM|_K$ of M over K splits as the direct sum $TM_K = E^s \oplus E^u$ of two DF -invariant vector bundles, where the vectors in E^s and E^u are uniformly contracted and expanded, respectively, by F^n , for some $n > 0$. Hyperbolic sets persist under small C^1 -perturbations of the dynamics: any diffeomorphism G which is C^1 -close enough to F admits a hyperbolic compact set K_G close to K and the restrictions of F and G to K and K_G are conjugated by a homeomorphism close to the identity. Hyperbolic compact sets have well-defined invariant (stable and unstable) manifolds, tangent (at the points of K) to E^s and E^u and the (local) invariant manifolds of K_G vary locally continuously with G .

The existence of hyperbolic sets is very common: if y is a transverse homoclinic point associated to a hyperbolic periodic point x , then there is a transitive hyperbolic set containing x and y .

Diffeomorphisms for which $\mathcal{R}(F)$ is hyperbolic are now well understood: the chain recurrence classes are homoclinic classes, finitely many, and transitive, and admit a combinatorial model (subshift of finite type). Some of them are

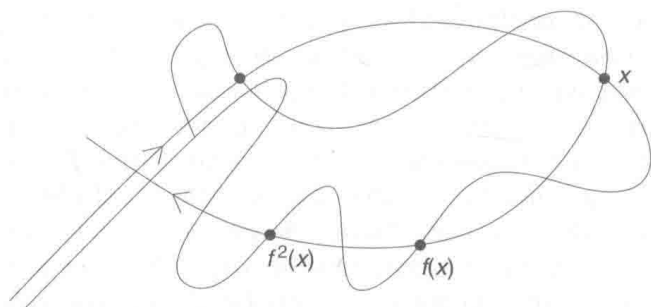


Figure 1 A transverse homoclinic orbit.

attractors or repellers, and the basins of the attractors cover a dense open subset of M . If, furthermore, all the stable and unstable manifolds of points in $\mathcal{R}(f)$ are transverse, the diffeomorphism is C^1 -structurally stable (Robbin 1971, Robinson 1976); indeed, this condition, called “axiom A + strong transversality,” is equivalent to the C^1 -structural stability (Mañé 1988).

In 1970, Abraham and Smale built examples of robustly non-axiom A diffeomorphisms, when $\dim M \geq 3$: the dream of a global understanding of dynamical systems was postponed. However, hyperbolicity remains a key tool in the study of dynamical systems, even for nonhyperbolic systems.

C^r -Generic Systems

Kupka–Smale Theorem

Thom’s transversality theorem asserts that two submanifolds can always be put in transverse position by a C^r -small perturbations. Hence, for F in an open and dense subset of $\text{Diff}^r(M)$, $r \geq 1$, the graph of F in $M \times M$ is transverse to the diagonal $\Delta = \{(x, x), x \in M\}$; F has finitely many fixed points x_i , depending locally continuously on F , and 1 is not an eigenvalue of the differential $DF(x_i)$. Small local perturbations in the neighborhood of the x_i avoid eigenvalue of modulus equal to 1: one gets a dense and open subset \mathcal{O}_1^r of $\text{Diff}^r(M)$ such that every fixed point is hyperbolic. This argument, adapted for periodic points, provides a dense and open set $\mathcal{O}_n^r \subset \text{Diff}^r(M)$, such that every periodic point of period n is hyperbolic. Now $\bigcap_{n \in \mathbb{N}} \mathcal{O}_n^r$ is a residual subset of $\text{Diff}^r(M)$, for which every periodic point is hyperbolic.

Similarly, the set of diffeomorphisms $F \in \bigcap_{i=0}^n \mathcal{O}_i^r(M)$ such that all the disks of size n , of invariant manifolds of periodic points of period less than n , are pairwise transverse, is open and dense. One gets the Kupka–Smale theorem (see Palis and de Melo (1982) for a detailed exposition): *for C^r -generic diffeomorphisms $F \in \text{Diff}^r(M)$, every periodic orbit is hyperbolic and $W^s(x)$ is transverse to $W^u(y)$ for $x, y \in \text{Per}(F)$.*

Generic Properties of Low-Dimensional Systems

Poincaré–Denjoy theory describes the topological dynamics of all diffeomorphisms of the circle S^1 (see Homeomorphisms and Diffeomorphisms of the Circle). Diffeomorphisms in an open and dense subset of $\text{Diff}_+^r(S^1)$ have a nonempty finite set of periodic orbits, all hyperbolic, and alternately attracting (sink) or repelling (source). The orbit of

a nonperiodic point comes from a source and goes to a sink. Two C^r -generic diffeomorphisms of S^1 are conjugated iff they have same rotation number and same number of periodic points.

This simple behavior has been generalized in 1962 by Peixoto for vector fields on compact orientable surfaces S . Vector fields X in a C^r -dense and open subset are Morse–Smale, hence structurally stable (see Palis and de Melo (1982) for a detailed proof). Peixoto gives a complete classification of these vector fields, up to topological equivalence.

Peixoto’s argument uses the fact that the return maps of the vector field on transverse sections are increasing functions: this helped control the effect on the dynamics of small “monotonous” perturbations, and allowed him to destroy any nontrivial recurrences. Peixoto’s result remains true on non-orientable surfaces for the C^1 -topology but remains an open question for $r > 1$: is the set of Morse–Smale vector fields C^2 -dense, for S nonorientable closed surface?

Local C^2 -Genericity of Wild Behavior for Surface Diffeomorphisms

The generic systems we have seen above have a very simple dynamics, simpler than the general systems. This is not always the case. In the 1970s, Newhouse exhibited a C^2 -open set $\mathcal{O} \subset \text{Diff}^2(S^2)$ (where S^2 denotes the two-dimensional sphere), such that C^2 -generic diffeomorphisms $F \in \mathcal{O}$ have infinitely many hyperbolic periodic sinks. In fact, C^2 -generic diffeomorphisms in \mathcal{O} present many other pathological properties: for instance, it has been recently noted that they have uncountably many chain recurrence classes without periodic orbits. Densely (but not generically) in \mathcal{O} , they present many other phenomena, such as strange (Henon-like) attractors (see Lyapunov Exponents and Strange Attractors).

This phenomenon appears each time that a diffeomorphism F_0 admits a hyperbolic periodic point x whose invariant manifolds $W^s(x)$ and $W^u(x)$ are tangent at some point $p \in W^s(x) \cap W^u(x)$ (p is a homoclinic tangency associated to x). Homoclinic tangencies appear locally as a codimension-1 submanifold of $\text{Diff}^2(S^2)$; they are such a simple phenomenon that they appear in very natural contexts. When a small perturbation transforms the tangency into transverse intersections, a new hyperbolic set K with very large fractal dimensions is created. The local stable and unstable manifolds of K , each homeomorphic to the product of a Cantor set by a segment, present tangencies in a C^2 -robust way, that is, for F in some C^2 -open set \mathcal{O} (see Figure 2). As a consequence, for a C^2 -dense subset of \mathcal{O} , the

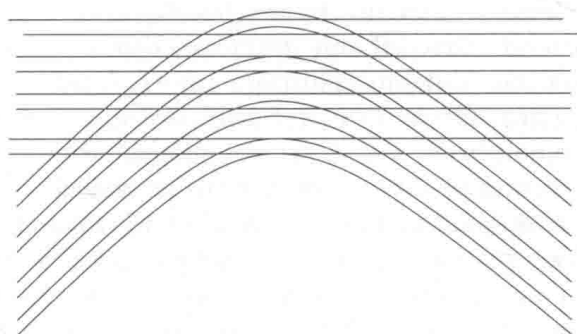


Figure 2 Robust tangencies.

invariant manifolds of the point x present some tangency (this is not generic, by Kupka–Smale theorem). If the Jacobian of F at x is < 1 , each tangency allows to create one more sink, by an arbitrarily small perturbation. Hence, the sets of diffeomorphisms having more than n hyperbolic sinks are dense open subsets of \mathcal{O} , and the intersection of all these dense open subsets is the announced residual set. See Palis and Takens (1993) for details on this deep argument.

C^1 -Generic Systems: Global Dynamics and Periodic Orbits

See Bonatti *et al.* (2004), Chapter 10 and Appendix A, for a more detailed exposition and precise references.

Perturbations of Orbits: Closing and Connecting Lemmas

In 1968, Pugh proved the following Lemma.

Closing lemma *If x is a nonwandering point of a diffeomorphism F , then there are diffeomorphisms G arbitrarily C^1 -close to F , such that x is periodic for G .*

Consider a segment $x_0, \dots, x_n = F^n(x_0)$ of orbit such that x_n is very close to $x_0 = x$; one would like to take G close to F such that $G(x_n) = x_0$, and $G(x_i) = F(x_i) = x_{i+1}$ for $i \neq n$. This idea works for the C^0 -topology (so that the C^0 -closing lemma is easy). However, if one wants G ε - C^1 -close to F , one needs that the points $x_i, i \in \{1, \dots, n-1\}$, remain at distance $d(x_i, x_0)$ greater than $C(d(x_n, x_0)/\varepsilon)$, where C bounds $\|Df\|$ on M . If C/ε is very large, such a segment of orbit does not exist. Pugh solved this difficulty in two steps: the perturbation is first spread along a segment of orbit of x in order to decrease this constant; then a subsegment y_0, \dots, y_k of x_0, \dots, x_n is selected, verifying the geometrical condition.

For the C^2 topology, the distances $d(x_i, x_0)$ need to remain greater than $\sqrt{d(x_n, x_0)}/\varepsilon \gg d(x_n, x_0)$. This new difficulty is why the C^2 -closing lemma remains an open question.

Pugh's argument does not suffice to create homoclinic point for a periodic orbit whose unstable manifold accumulates on the stable one. In 1998, Hayashi solved this problem proving the

Connecting lemma (Hayashi 1997) *Let y and z be two points such that the forward orbit of y and the backward orbit of z accumulate on the same nonperiodic point x . Fix some $\varepsilon > 0$. There is $N > 0$ and a ε - C^1 -perturbation G of F such that $G^n(y) = z$ for some $n > 0$, and $G \equiv F$ out of an arbitrary small neighborhood of $\{x, F(x), \dots, F^N(x)\}$.*

Using Hayashi's arguments, we (with Crovisier) proved the following lemma:

Connecting lemma for pseudo-orbits (Bonatti and Crovisier 2004) *Assume that all periodic orbits of F are hyperbolic; consider $x, y \in M$ such that, for any $\varepsilon > 0$, there are ε -pseudo-orbits joining x to y ; then there are arbitrarily small C^1 -perturbations of F for which the positive orbit of x passes through y .*

Densities of Periodic Orbits

As a consequence of the perturbations lemma above, we (Bonatti and Crovisier 2004) proved that for F C^1 -generic,

$$\mathcal{R}(F) = \Omega(F) = \overline{\text{Per}_{\text{hyp}}(F)}$$

where $\overline{\text{Per}_{\text{hyp}}(F)}$ denotes the closure of the set of hyperbolic periodic points.

For this, consider the map $\Psi: F \mapsto \Psi(F) = \overline{\text{Per}_{\text{hyp}}(F)}$ defined on $\text{Diff}^1(M)$ and with value in $\mathcal{K}(M)$, space of all compact subsets of M , endowed with the Hausdorff topology. $\text{Per}_{\text{hyp}}(F)$ may be approximated by a finite set of hyperbolic periodic points, and this set varies continuously with F ; so $\text{Per}_{\text{hyp}}(F)$ varies lower-semicontinuously with F : for G very close to F , $\text{Per}_{\text{hyp}}(G)$ cannot be very much smaller than $\text{Per}_{\text{hyp}}(F)$. As a consequence, a result from general topology asserts that, for C^1 -generic F , the map Ψ is continuous at F . On the other hand, C^1 -generic diffeomorphisms are Kupka–Smale, so that the connecting lemma for pseudo-orbits may apply: if $x \in \mathcal{R}(F)$, x can be turned into a hyperbolic periodic point by a C^1 -small perturbation of F . So, if $x \notin \overline{\text{Per}_{\text{hyp}}(F)}$, F is not a continuity point of Ψ , leading to a contradiction.

Furthermore, Crovisier proved the following result: “for C^1 -generic diffeomorphisms, each chain recurrence class is the limit, for the Hausdorff distance, of a sequence of periodic orbits.”

This good approximation of the global dynamics by the periodic orbits will now allow us to better understand the chain recurrence classes of C^1 -generic diffeomorphisms.

Chain Recurrence Classes/Homoclinic Classes of C^1 -Generic Systems

Transverse intersections of invariant manifolds of hyperbolic orbits are robust and vary locally continuously with the diffeomorphisms F . So, the homoclinic class $H(x)$ of a periodic point x varies lower-semicontinuously with F (on the open set where the continuation of x is defined). As a consequence, for C^r -generic diffeomorphisms ($r \geq 1$), each homoclinic class varies continuously with F . Using the connecting lemma, Arnaud (2001) proved the following result: “for Kupka–Smale diffeomorphisms, if the closures $\overline{W}_{\text{orb}}^u(x)$ and $\overline{W}_{\text{orb}}^s(x)$ have some intersection point z , then a C^1 -perturbation of F creates a transverse intersection of $\overline{W}_{\text{orb}}^u(x)$ and $\overline{W}_{\text{orb}}^s(x)$ at z .” So, if $z \notin H(x)$, then F is not a continuity point of the function $F \mapsto H(x, F)$. Hence, for C^1 -generic diffeomorphisms F and for every periodic point x ,

$$H(x) = \overline{W}_{\text{orb}}^u(x) \cap \overline{W}_{\text{orb}}^s(x)$$

In the same way, $\overline{W}_{\text{orb}}^u(x)$ and $\overline{W}_{\text{orb}}^s(x)$ vary locally lower-semicontinuously with F so that, for F C^r -generic, the closures of the invariant manifolds of each periodic point vary locally continuously. For Kupka–Smale diffeomorphisms, the connecting lemma for pseudo-orbits implies: “if z is a point in the chain recurrence class of a periodic point x , then a C^1 -small perturbation of F puts z on the unstable manifold of x ”; so, if $z \notin \overline{W}_{\text{orb}}^u(x)$, then F is not a continuity point of the function $F \mapsto \overline{W}_{\text{orb}}^u(x, F)$. Hence, for C^1 -generic diffeomorphisms F and for every periodic point x , the chain recurrence class of x is contained in $\overline{W}_{\text{orb}}^u(x) \cap \overline{W}_{\text{orb}}^s(x)$, and, therefore, coincides with the homoclinic class of x . This argument proves:

For a C^1 -generic diffeomorphism F , each homoclinic class $H(x)$ is a chain recurrence class of F (of Conley’s theory): a chain recurrence class containing a periodic point x coincides with the homoclinic class $H(x)$. In particular, two homoclinic classes are either disjoint or equal.

Tame and Wild Systems

For generic diffeomorphisms, the number $N(F) \in \mathbb{N} \cup \{\infty\}$ of homoclinic classes varies lower-semicontinuously with F . One deduces that $N(F)$ is locally constant on a residual subset of $\text{Diff}^1(M)$ (Abdenur 2003).

A local version (in the neighborhood of a chain recurrence class) of this argument shows that, for C^1 -generic diffeomorphisms, any isolated chain recurrence class C is robustly isolated: for any diffeomorphism G , C^1 -close enough to F , the intersection of $\mathcal{R}(G)$ with a small neighborhood of C is a unique chain recurrence class C_G close to C .

One says that a diffeomorphism is “tame” if each chain recurrence class is robustly isolated. We denote by $\mathcal{T}(M) \subset \text{Diff}^1(M)$ the (C^1 -open) set of tame diffeomorphisms and by $\mathcal{W}(M)$ the complement of the closure of $\mathcal{T}(M)$. C^1 -generic diffeomorphisms in $\mathcal{W}(M)$ have infinitely many disjoint homoclinic classes, and are called “wild” diffeomorphisms.

Generic tame diffeomorphisms have a global dynamics analogous to hyperbolic systems: the chain recurrence set admits a partition into finitely many homoclinic classes varying continuously with the dynamics. Every point belongs to the stable set of one of these classes. Some of the homoclinic classes are (transitive) topological attractors, and the union of the basins covers a dense open subset of M , and the basins vary continuously with F (Carballo Morales 2003). It remains to get a good description of the dynamics in the homoclinic classes, and particularly in the attractors. As we shall see in the next section, tame behavior requires some kind of weak hyperbolicity. Indeed, in dimension 2, tame diffeomorphisms satisfy axiom A and the noncycle condition.

As of now, very little is known about wild systems. One knows some semilocal mechanisms generating locally C^1 -generic wild dynamics, therefore proving their existence on any manifold with dimension $\dim(M) \geq 3$ (the existence of wild diffeomorphisms in dimension 2, for the C^1 -topology, remains an open problem). Some of the known examples exhibit a universal dynamics: they admit infinitely many disjoint periodic disks such that, up to renormalization, the return maps on these disks induce a dense subset of diffeomorphisms of the disk. Hence, these locally generic diffeomorphisms present infinitely many times any robust property of diffeomorphisms of the disk.

Ergodic Properties

A point x is well closable if, for any $\varepsilon > 0$ there is $G \varepsilon$ - C^1 -close to F such that x is periodic for G and $d(F^i(x), G^i(x)) < \varepsilon$ for $i \in \{0, \dots, p\}$, p being the period of x . As an important refinement of Pugh’s closing lemma, Mañé proved the following lemma:

Ergodic closing lemma For any F -invariant probability, almost every point is well closable.

As a consequence, “for C^1 -generic diffeomorphisms, any ergodic measure μ is the weak limit of a sequence of Dirac measures on periodic orbits, which converges also in the Hausdorff distance to the support of μ .”

It remains an open problem to know if, for C^1 -generic diffeomorphisms, the ergodic measures supported in a homoclinic class are approached by periodic orbits in this homoclinic class.

Conservative Systems

The connecting lemma for pseudo-orbits has been adapted for volume preserving and symplectic diffeomorphisms, replacing the condition on the periodic orbits by another generic condition on the eigenvalues. As a consequence, one gets: “ C^1 -generic volume-preserving or symplectic diffeomorphisms are transitive, and M is a unique homoclinic class.”

Notice that the KAM theory implies that this result is wrong for C^4 -generic diffeomorphisms, the persistence of invariant tori allowing to break robustly the transitivity.

The Oxtoby–Ulam (1941) theorem asserts that C^0 -generic volume-preserving homeomorphisms are ergodic. The ergodicity of C^1 -generic volume-preserving diffeomorphisms remains an open question.

Hyperbolic Properties of C^1 -Generic Diffeomorphisms

For a more detailed exposition of hyperbolic properties of C^1 -generic diffeomorphisms, the reader is referred to Bonatti *et al.* (2004, chapter 7 and appendix B).

Perturbations of Products of Matrices

The C^1 -topology enables us to do small perturbations of the differential DF at a point x without perturbing either $F(x)$ or F out of an arbitrarily small neighborhood of x . Hence, one can perturb the differential of F along a periodic orbit, without changing this periodic orbit (Frank’s lemma). When x is a periodic point of period n , the differential of F^n at x is fundamental for knowing the local behavior of the dynamics. This differential is (up to a choice of local coordinates) a product of the matrices $DF(x_i)$, where $x_i = F^i(x)$. So, the control of the dynamical effect of local perturbations along a periodic orbit comes from a problem of linear algebra: “consider a product $A = A_n \circ A_{n-1} \circ \cdots \circ A_1$ of $n \gg 0$ bounded linear isomorphisms of \mathbb{R}^d ; how do the eigenvalues and the eigenspaces of A vary under small perturbations of the A_i ?”

A partial answer to this general problem uses the notion of dominated splitting. Let $X \subset M$ be an

F -invariant set such that the tangent space of M at the points $x \in X$ admits a DF -invariant splitting $T_x(M) = E_1(x) \oplus \cdots \oplus E_k(x)$, the dimensions $\dim(E_i(x))$ being independent of x . This splitting is dominated if the vectors in E_{i+1} are uniformly more expanded than the vectors in E_i : there exists $\ell > 0$ such that, for any $x \in X$, any $i \in \{1, \dots, k-1\}$ and any unit vectors $u \in E_i(x)$ and $v \in E_{i+1}(x)$, one has

$$\|DF^\ell(u)\| < \frac{1}{2} \|DF^\ell(v)\|$$

Dominated splittings are always continuous, extend to the closure of X , and persist and vary continuously under C^1 -perturbation of F .

Dominated Splittings versus Wild Behavior

Let $\{\gamma_i\}$ be a set of hyperbolic periodic orbits. On $X = \bigcup \gamma_i$ one considers the natural splitting $TM|_X = E^s \oplus E^u$ induced by the hyperbolicity of the γ_i . Mañé (1982) proved: “if there is a C^1 -neighborhood of F on which each γ_i remains hyperbolic, then the splitting $TM|_X = E^s \oplus E^u$ is dominated.”

A generalization of Mañé’s result shows: “if a homoclinic class $H(x)$ has no dominated splitting, then for any $\varepsilon > 0$ there is a periodic orbit γ in $H(x)$ whose derivative at the period can be turned into an homothety, by an ε -small perturbation of the derivative of F along the points of γ ”; in particular, this periodic orbit can be turned into a sink or a source. As a consequence, one gets: “for C^1 -generic diffeomorphisms F , any homoclinic class either has a dominated splitting or is contained in the closure of the (infinite) set of sinks and sources.”

This argument has been used in two directions:

- Tame systems must satisfy some hyperbolicity. In fact, using the ergodic closing lemma, one proves that the homoclinic classes $H(x)$ of tame diffeomorphisms are volume hyperbolic, that is, there is a dominated splitting $TM = E_1 \oplus \cdots \oplus E_k$ over $H(x)$ such that DF contracts uniformly the volume in E_1 and expands uniformly the volume in E_k .
- If F admits a homoclinic class $H(x)$ which is robustly without dominated splittings, then generic diffeomorphisms in the neighborhood of F are wild: at this time this is the unique known way to get wild systems.

See also: Cellular Automata; Chaos and Attractors; Fractal Dimensions in Dynamics; Homeomorphisms and Diffeomorphisms of the Circle; Homoclinic Phenomena; Hyperbolic Dynamical Systems; Lyapunov Exponents and Strange Attractors; Polygonal Billiards; Singularity and Bifurcation Theory; Synchronization of Chaos.

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Geometric Analysis and General Relativity

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Geometric analysis can be said to originate in the nineteenth century work of Weierstrass, Riemann, Schwarz, and others on minimal surfaces, a problem whose history can be traced at least as far back as the work of Meusnier and Lagrange in the eighteenth century. The experiments performed by Plateau in the mid-19th century, on soap films spanning wire contours, served as an important inspiration for this work, and led to the formulation of the Plateau problem, which concerns the existence and regularity of area-minimizing surfaces in \mathbb{R}^3 spanning a given boundary contour. The Plateau problem for area-minimizing disks spanning a curve in \mathbb{R}^3 was solved by J Douglas (who shared the first Fields medal with Lars V Ahlfors) and T Rado in the 1930s. Generalizations of Plateau's problem have been an important driving force behind the development of modern geometric analysis. Geometric analysis can be viewed broadly as the study of partial differential equations arising in geometry, and includes many areas of the calculus of variations, as well as the theory of geometric evolution equations. The Einstein equation, which is the central object of general relativity, is one of the most widely studied geometric partial differential equations, and plays an important role in its Riemannian as well as in its Lorentzian form, the Lorentzian being most relevant for general relativity.

The Einstein equation is the Euler–Lagrange equation of a Lagrangian with gauge symmetry and thus in the Lorentzian case it, like the Yang–Mills equation, can be viewed as a system of evolution equations with constraints. After imposing suitable gauge conditions, the Einstein equation becomes a hyperbolic system, in particular using spacetime harmonic coordinates (also known as wave coordinates), the Einstein equation becomes a quasilinear system of wave equations. The constraint equations implied by the Einstein equations can be viewed as a system of elliptic equations in terms of suitably chosen variables. Thus, the Einstein equation leads to both elliptic and hyperbolic problems, arising from the constraint equations and the Cauchy problem, respectively. The groundwork for the mathematical study of the Einstein equation and the global nature of spacetimes was laid by, among others, Choquet-Bruhat, who proved local well-posedness for the Cauchy problem, Lichnerowicz, and later York who provided the basic ideas for the analysis of the constraint equations, and Leray who formalized the notion of global hyperbolicity, which is essential for the global study of spacetimes. An important framework for the mathematical study of the Einstein equations has been provided by the singularity theorems of Penrose and Hawking, as well as the cosmic censorship conjectures of Penrose.

Techniques and ideas from geometric analysis have played, and continue to play, a central role in recent mathematical progress on the problems posed by general relativity. Among the main results are the

proof of the positive mass theorem using the minimal surface technique of Schoen and Yau, and the spinor-based approach of Witten, as well as the proofs of the (Riemannian) Penrose inequality by Huisken and Illmanen, and Bray. The proof of the Yamabe theorem by Schoen has played an important role as a basis for constructing Cauchy data using the conformal method.

The results just mentioned are all essentially Riemannian in nature, and do not involve study of the Cauchy problem for the Einstein equations. There has been great progress recently concerning global results on the Cauchy problem for the Einstein equations, and the cosmic censorship conjectures of Penrose. The results available so far are either small data results (among these the nonlinear stability of Minkowski space proved by Christodoulou and Klainerman) or assume additional symmetries, such as the recent proof by Ringström of strong cosmic censorship for the class of Gowdy spacetimes. However, recent progress concerning quasi-linear wave equations and the geometry of spacetimes with low regularity due to, among others, Klainerman and Rodnianski, and Tataru and Smith, appears to show the way towards an improved understanding of the Cauchy problem for the Einstein equations.

Since the constraint equations, the Penrose inequality and the Cauchy problem are discussed in separate articles, the focus of this article will be on the role in general relativity of “critical” and other geometrically defined submanifolds and foliations, such as minimal surfaces, marginally trapped surfaces, constant mean curvature hypersurfaces and null hypersurfaces. In this context it would be natural also to discuss geometrically defined flows such as mean curvature flows, inverse mean curvature flow, and Ricci flow. However, this article restricts the discussion to mean curvature flows, since the inverse mean curvature flow appears naturally in the context of the Penrose inequality and the Ricci flow has so far mainly served as a source of inspiration for research on the Einstein equations rather than an important tool. Other topics which would fit well under the heading “General relativity and geometric analysis” are spin geometry (the Witten proof of the Positive mass theorem), the Yamabe theorem and related results concerning the Einstein constraint equations, gluing and other techniques of “spacetime engineering.” These are all discussed in other articles. Some techniques which have only recently come into use and for which applications in general relativity have not been much explored, such as Cheeger–Gromov compactness, are not discussed.

Minimal and Related Surfaces

Consider a hypersurface N in Euclidean space \mathbb{R}^n which is a graph $x_n = u(x_1, \dots, x_{n-1})$ with respect to the function u . The area of N is given by $A(N) = \int \sqrt{1 + |Du|^2} dx^1 \cdots dx^{n-1}$. N is stationary with respect to A if u satisfies the equation

$$\sum_i D_i \left(\frac{D_i u}{\sqrt{1 + |Du|^2}} \right) = 0 \quad [1]$$

A hypersurface N defined as a graph of u solving [1] minimizes area with respect to compactly supported deformations, and hence is called a minimal surface. For $n \leq 7$, a solution to eqn [1] defined on all of \mathbb{R}^{n-1} must be an affine function. This fact is known as a Bernstein principle. Equation [1], and more generally, the prescribed mean curvature equation which will be discussed below, is a quasi-linear, uniformly elliptic second-order equation. The book by Gilbarg and Trudinger (1983) is an excellent general reference for such equations.

The theory of rectifiable currents, developed by Federer and Fleming, is a basic tool in the modern approach to the Plateau problem and related variational problems. A rectifiable current is a countable union of Lipschitz submanifolds, counted with integer multiplicity, and satisfying certain regularity conditions. Hausdorff measure gives a notion of area for these objects. One may therefore approach the study of minimal surfaces via rectifiable currents which are stationary with respect to variations of area. Suitable generalizations of familiar notions from smooth differential geometry such as tangent plane, normal vector, extrinsic curvature can be introduced. The book by Federer (1969) is a classic treatise on the subject. Further information concerning minimal surfaces and related variational problems can be found in Lawson, Jr. (1980) and Simon (1997). Note, however, that unless otherwise stated, all fields and manifolds considered in this article are assumed to be smooth. For the Plateau problem in a Riemannian ambient space, we have the following existence and regularity result.

Theorem 1 (Existence of embedded solutions for Plateau problem). *Let M be a complete Riemannian manifold of dimension $n \leq 7$ and let Γ be a compact $(n - 2)$ -dimensional submanifold in M which bounds. Then there is an $(n - 1)$ -dimensional area-minimizing hypersurface N with Γ as its boundary. N is a smooth, embedded manifold in its interior.*

If the dimension of the ambient space is > 7 , solutions to the Plateau problem will in general have a singular set of dimension $n - 8$. Let N be an oriented hypersurface of a Riemannian manifold M

with covariant derivative D . Let η be the unit normal of N and define the second fundamental form and mean curvature of N by $A_{ij} = \langle D_{e_i} \eta, e_j \rangle$ and $H = \text{tr} A$. Define the action functional $\mathcal{E}(N) = \mathcal{A}(N) - \int_{M;N} H_0$, where H_0 is a function defined on M , and $\int_{M;N}$ denotes the integral over the volume bounded by N in M . The problem of minimizing \mathcal{E} is a useful generalization of the minimization problem for \mathcal{A} .

Theorem 2 (Existence of minimizers in homology). *Let M be a compact Riemannian manifold of dimension ≤ 7 , and let α be an integral homology class on M of codimension 1. Then there is a smooth minimizer for \mathcal{E} representing $[\alpha]$.*

Again, in higher dimensions, the minimizers will in general have singularities. The general form of this result deals with elliptic functionals. For surfaces in 3-manifolds, the problem of minimizing area within homotopy classes has been studied. Results in this direction played a central role in the approach of Schoen and Yau to manifolds with non-negative scalar curvature.

If M is not compact, it is in general necessary to use barriers to control the minimizers, or consider some version of the Plateau problem. Barriers can be used due to the strong maximum principle, which holds for the mean curvature operator since it is quasilinear elliptic. Consider two hypersurfaces N_1, N_2 which intersect at a point p and assume that N_1 lies on one side of N_2 with the normal pointing towards N_1 . If the mean curvatures H_1, H_2 of the hypersurfaces, defined with respect to consistently oriented normals, satisfy $H_1 \leq \lambda \leq H_2$ for some constant λ , then N_1 and N_2 coincide near p and have mean curvatures equal to λ . This result requires only mild regularity conditions on the hypersurfaces. Generalizations hold also for the case of spacelike or null hypersurfaces in a Lorentzian ambient space, see Andersson *et al.* (1998) and Galloway (2000).

Let ϕ be a smooth compactly supported function on N . The variation $\mathcal{E}' = \delta_{\phi\eta} \mathcal{E}$ of \mathcal{E} under a deformation $\phi\eta$ is

$$\mathcal{E}' = \int_N \phi(H - H_0)$$

Thus, N is stationary with respect to \mathcal{E} if and only if N solves the prescribed mean curvature equation $H(x) = H_0(x)$ for $x \in N$. Supposing that N is stationary and H_0 is constant, the second variation $\mathcal{E}'' = \delta_{\phi\eta} \mathcal{E}'$ of \mathcal{E} is of the form

$$\mathcal{E}'' = \int_N \phi(J\phi)$$

where J is the second-variation operator, a second-order elliptic operator. A calculation, using the

Gauss equation and the second-variation equation shows

$$J\phi = -\Delta_N \phi - \frac{1}{2}[(\text{Scal}_M - \text{Scal}_N) + H^2 + |A|^2]\phi \quad [2]$$

where $\Delta_N, \text{Scal}_M, \text{Scal}_N$ denote the Laplace–Beltrami operator of N , and the scalar curvatures of M and N , respectively. If J is positive semidefinite, N is called stable.

To set the context where we will apply the above, let (M, g_{ij}) be a connected, asymptotically Euclidean three-dimensional Riemannian manifold with covariant derivative, and let k_{ij} be a symmetric tensor on M . Suppose (M, g_{ij}, K_{ij}) is imbedded isometrically as a spacelike hypersurface in a space-time $(V, \gamma_{\alpha\beta})$ with g_{ij}, K_{ij} the first and second fundamental forms induced on M from V , in particular $K_{ij} = \langle D_{e_i} T, e_j \rangle$ where T is the timelike normal of M in the ambient spacetime V , and D is the ambient covariant derivative. We will refer to (M, g_{ij}, K_{ij}) as a Cauchy data set for the Einstein equations. Although many of the results which will be discussed below generalize to the case of a nonzero cosmological constant Λ , we will discuss only the case $\Lambda = 0$ in this article. $G_{\alpha\beta} = \text{Ric}_{V\alpha\beta} - (1/2)\text{Scal}_V \gamma_{\alpha\beta}$ be the Einstein tensor of V , and let $\rho = G_{\alpha\beta} T^\alpha T^\beta, \mu_i = G_{j\alpha} T^\alpha$. Then the fields (g_{ij}, K_{ij}) satisfy the Einstein constraint equations

$$R + \text{tr } K^2 - |K|^2 = 2\rho \quad [3]$$

$$\nabla_j \text{tr } K - \nabla^i K_{ij} = \mu_j \quad [4]$$

We assume that the dominant energy condition (DEC)

$$\rho \geq \left(\sum_i \mu_i \mu^i \right)^{1/2} \quad [5]$$

holds. We will sometimes make use of the null energy condition (NEC), $G_{\alpha\beta} L^\alpha L^\beta \geq 0$ for null vectors L , and the strong energy condition (SEC), $\text{Ric}_{V\alpha\beta} v^\alpha v^\beta \geq 0$ for causal vectors v . M will be assumed to satisfy the fall-off conditions

$$g_{ij} = \left(1 + \frac{2m}{r} \right) \delta_{ij} + O(1/r^2) \quad [6a]$$

$$K_{ij} = O(1/r^2) \quad [6b]$$

as well as suitable conditions for the fall-off of derivatives of g_{ij}, K_{ij} . Here m is the ADM (Arnowitt, Deser, Misner) mass of (M, g_{ij}, K_{ij}) .

Minimal Surfaces and Positive Mass

Perhaps the most important application of the theory of minimal surfaces in general relativity is in the

Schoen–Yau proof of the positive-mass theorem, which states that $m \geq 0$, and $m = 0$ only if (M, g, K) can be embedded as a hypersurface in Minkowski space. Consider an asymptotically Euclidean manifold (M, g) with g satisfying [6a] and with non-negative scalar curvature. By using Jang's equation, see below, the general situation is reduced to the case of a time symmetric data set, with $K = 0$. In this case, the DEC implies that (M, g) has non-negative scalar curvature.

Assuming $m < 0$ one may, after applying a conformal deformation, assume that $\text{Scal}_M > 0$ in the complement of a compact set. Due to the asymptotic conditions, level sets for sufficiently large values of one of the coordinate functions, say x^3 , can be used as barriers for minimal surfaces in M . By solving a sequence of Plateau problems with boundaries tending to infinity, a stable entire minimal surface N homeomorphic to the plane is constructed. Stability implies using [2],

$$\int_N \left(\frac{1}{2} \text{Scal}_M - \kappa + \frac{1}{2} |A|^2 \right) \leq 0$$

where $\kappa = (1/2)\text{Scal}_N$ is the Gauss curvature of N . Since by construction $\text{Scal}_M \geq 0$, $\text{Scal}_M > 0$ outside a compact set, this gives $\int_N \kappa > 0$. Next, one uses the identity, related to the Cohn–Vossen inequality

$$\int_N \kappa = 2\pi - \lim_i \frac{L_i^2}{2A_i}$$

where A_i, L_i are the area and circumference of a sequence of large discs. Estimates using the fact that M is asymptotically Euclidean show that $\lim_i (L_i^2/2A_i) \geq 2\pi$ which gives a contradiction and shows that the minimal surface constructed cannot exist. It follows that $m \geq 0$. It remains to show that the case $m = 0$ is rigid. To do this proves that for an asymptotically Euclidean metric with non-negative scalar curvature, which is positive near infinity, there is a conformally related metric with vanishing scalar curvature and strictly smaller mass. Applying this argument in case $m = 0$ gives a contradiction to the fact that $m \geq 0$. Therefore, $m = 0$ only if the scalar curvature vanishes identically. Suppose now that (M, g) has vanishing scalar curvature but nonvanishing Ricci curvature Ric_M . Then using a deformation of g in the direction of Ric_M , one constructs a metric close to g with negative mass, which leads to a contradiction.

This technique generalizes to Cauchy surfaces of dimension $n \leq 7$. The proof involves induction on dimension. For $n > 7$ minimal hypersurfaces are singular in general and this approach runs into problems. The Witten proof using spinor techniques does not suffer from this limitation but instead requires that M be spin.

Marginally Trapped Surfaces

Consider a Cauchy data set (M, g_{ij}, K_{ij}) as above and let N be a compact surface in M with normal η , second fundamental form A and mean curvature H . Then considering N as a surface in an ambient Lorentzian space V containing M , N has two null normal fields which after a rescaling can be taken to be $L_{\pm} = T \pm \eta$. Here, T is the future-directed time-like unit normal of M in V . The null mean curvatures (or null expansions) corresponding to L_{\pm} can be defined in terms of the variation of the area element μ_N of N as $\delta_{L_{\pm}} \mu_N = \theta_{\pm} \mu_N$ or

$$\theta_{\pm} = \text{tr}_N K \pm H$$

where $\text{tr}_N K$ denotes the trace of the projection of K_{ij} to N . Suppose L_+ is the outgoing null normal. N is called outer trapped (marginally trapped, untrapped) if $\theta_+ < 0$ ($\theta_+ = 0$, $\theta_+ > 0$). An asymptotically flat spacetime which contains a trapped surface with $\theta_- < 0$, $\theta_+ < 0$ is causally incomplete. In the following we will for simplicity drop the word outer from our terminology.

Consider a Cauchy surface M . The boundary of the region in M containing trapped surfaces is, if it is sufficiently smooth, a marginally trapped surface. The equation $\theta_+ = 0$ is an equation analogous to the prescribed curvature equation, in particular it is a quasilinear elliptic equation of second order. Marginally trapped surfaces are not variational in the same sense as minimal surfaces. Nevertheless, they are stationary with respect to variations of area within the outgoing light cone. The second variation of area along the outgoing null cone is given, in view of the Raychaudhuri equation, by

$$\delta_{\phi L_+} \theta_+ = -(G_{++} + |\sigma_+|^2) \phi \quad [7]$$

for a function ϕ on N . Here $G_{++} = G_{\alpha\beta} L_+^{\alpha} L_+^{\beta}$, and σ_+ denotes the shear of N with respect to L_+ , that is, the tracefree part of the null second fundamental form with respect to L_+ . Equation [7] shows that the stability operator in the direction L_+ is not elliptic.

In the case of time-symmetric data, $K_{ij} = 0$, the DEC implies $\text{Scal}_M \geq 0$ and marginally trapped surfaces are simply minimal surfaces. A stable compact minimal 2-surface N in a 3-manifold M with non-negative scalar curvature must satisfy

$$2\pi\chi(N) = \int \kappa \geq \frac{1}{2} \int_N \text{Scal}_M + |A|^2 \geq 0$$

and hence by the Gauss–Bonnet theorem, N is diffeomorphic to a sphere or a torus. In case N is a stable minimal torus, the induced geometry is flat and the ambient curvature vanishes at N . If, in addition, N minimizes, then M is flat.

For a compact marginally trapped surface N in M , analogous results can be proved by studying the stability operator defined with respect to the direction η . Let J be the operator defined in terms of a variation of θ_+ by $J\phi = \delta_{\phi\eta}\theta_+$. Then

$$J\phi = -\Delta_N\phi + 2s^A D_A\phi + \left(\frac{1}{2} \text{Scal}_N - s_A s^A + D_A s^A - \frac{1}{2} |\sigma_+|^2 - G_{+-}\right)\phi$$

Here, $s_A = -(1/2)\langle L_-, D_A L_+ \rangle$ and G_{+-} is the Einstein tensor evaluated on L_+, L_- . We may call N stable if the real part of the spectrum of J is non-negative. A sufficient condition for N to be stable is that N is locally outermost. This can be formulated, for example, by requiring that a neighborhood of N in M contains no trapped surfaces exterior to N . In this case, assuming that the DEC holds, N is a sphere or a torus, and if the real part of the spectrum of J is positive then N is a sphere. If N is a torus, then the ambient curvature and shear vanishes at N , s_A is a gradient, and N is flat. One expects that in addition, global rigidity should hold, in analogy with the minimal surface case. This is an open problem. If N satisfies the stronger condition of strict stability, which corresponds to the spectrum of J having positive real part, then N is in the interior of a hypersurface H of the ambient spacetime, with the property that it is foliated by marginally trapped surfaces (Andersson *et al.* 2005). If the NEC holds and N has nonvanishing shear, then H is spacelike at N . A hypersurface H with these properties is known as a dynamical horizon.

Jang's Equation

Consider a Cauchy data set (M, g_{ij}, K_{ij}) . Extend K_{ij} to a tensor field on $M \times \mathbb{R}$, constant in the vertical direction. Then the equation for a graph

$$N = \{(x, t) \in M \times \mathbb{R}, \quad t = f(x)\}$$

such that N has mean curvature equal to the trace of the projection of K_{ij} to N with respect to the induced metric on N , is given by

$$\sum_{ij} \left(K^{ij} - \frac{\nabla^i \nabla^j f}{(1 + |\nabla f|^2)^{1/2}} \right) \left(g_{ij} - \frac{\nabla_i f \nabla_j f}{1 + |\nabla f|^2} \right) = 0 \quad [8]$$

an equation closely related to the equation $\theta_+ = 0$. Equation [8] was introduced by P S Jang (Jang 1978) as part of an attempt to generalize the inverse mean curvature flow method of Geroch from time-symmetric to general Cauchy data.

Existence and regularity for Jang's equation were proved by Schoen and Yau (1981) and used to

generalize their proof of the positive-mass theorem from the case of maximal slices to the general case. The solution to Jang's equation is constructed as the limit of the solution to a sequence of regularized problems. The limit consists of a collection N of submanifolds of $M \times \mathbb{R}$. In particular, component near infinity is a graph and has the same mass as M . N may contain vertical components which project onto marginally trapped surfaces in M , and in fact these constitute the only possibilities for blow-up of the sequence of graphs used to construct N . If the DEC is valid, the metric on N has non-negative scalar curvature in the weak sense that

$$\int_N \text{Scal}_N \phi^2 + 2|\nabla \phi|^2 > 0$$

for smooth compactly supported functions ϕ . If the DEC holds strictly, the strict inequality holds and in this case the metric on N is conformal to a metric with vanishing scalar curvature.

Jang's equation can be applied to prove existence of marginally trapped surfaces, given barriers. Let (M, g_{ij}, K_{ij}) be a Cauchy data set containing two compact surfaces N_1, N_2 which together bound a compact region M' in M . Suppose the surfaces N_1 and N_2 have $\theta_+ < 0$ on N_1 and $\theta_+ > 0$ on N_2 . Schoen recently proved the following result.

Theorem 3 (Existence of marginally trapped surfaces). *Let M', N_1, N_2 be as above. Then there is a finite collection of compact, marginally trapped surfaces $\{\Sigma_a\}$ contained in the interior of M' , such that $\cup \Sigma_a$ is homologous to N_1 . If the DEC holds, then Σ_a is a collection of spheres and tori.*

The proof proceeds by solving a sequence of Dirichlet boundary-value problems for Jang's equation with boundary value on N_1, N_2 tending to $-\infty$ and ∞ , respectively. The assumption on θ_+ is used to show the existence of barriers for Jang's equation. Let f_k be the sequence of solutions to the Dirichlet problems. Jang's equation is invariant under renormalization $f_k \rightarrow f_k + c_k$ for some sequence c_k of real numbers. A Harnack inequality for the gradient of the solutions to Jang's equation is used to show that the sequence of solutions f_k , possibly after a renormalization, has a subsequence converging to a vertical submanifold of $M' \times \mathbb{R}$, which projects to a collection Σ_a of marginally trapped surfaces. By construction, the zero sets of the f_k are homologous to N_1 and N_2 . The estimates on the sequence $\{f_k\}$ show that this holds also in the limit $k \rightarrow \infty$. The statement about the topology of the Σ_a follows by showing, using the above-mentioned inequality for Scal_N , that if DEC holds, the total Gauss curvature of each surface Σ_a is non-negative.

Center of mass

Since by the positive-mass theorem $m > 0$ unless the ambient spacetime is flat, it makes sense to consider the problem of finding an appropriate notion of center of mass. This problem was solved by Huisken and Yau who showed that under the asymptotic conditions [6] the isoperimetric problem has a unique solution if one considers sufficiently large spheres.

Theorem 4 (Huisken and Yau 1996). *There is an $H_0 > 0$ and a compact region B_{H_0} such that for each $H \in (0, H_0)$ there is a unique constant mean curvature sphere S_H with mean curvature H contained in $M \setminus B_{H_0}$. The spheres form a foliation.*

The proof involves a study of the evolution equation

$$\frac{dx}{ds} = (H - \bar{H})\eta \quad [9]$$

where \bar{H} is the average mean curvature. This is the gradient flow for the isoperimetric problem of minimizing area keeping the enclosed volume constant. The solutions in Euclidean space are standard spheres. Equation [9] defines a parabolic system, in particular we have

$$\frac{d}{ds}H = \Delta H + (\text{Ric}(\eta, \eta) + |A|^2)(H - \bar{H})$$

It follows from the fall-off conditions [6] that the foliation of spheres constructed in Theorem 4 are untrapped surfaces. They can therefore be used as outer barriers in the existence result for marginally trapped surfaces, (Theorem 3).

The mean curvature flow for a spatial hypersurface in a Lorentz manifold is also parabolic. This flow has been applied to construct constant mean curvature Cauchy hypersurfaces in spacetimes.

Maximal and Related Surfaces

Let N be the hypersurface $x_0 = u(x_1, \dots, x_n)$ in Minkowski space \mathbb{R}^{1+n} with line element $-dx_0^2 + dx_1^2 + \dots + dx_n^2$. Assume $|\nabla u| < 1$ so that N is spacelike. Then N is stationary with respect to variations of area if u solves the equation

$$\sum_i \nabla_i \left(\frac{\nabla_i u}{\sqrt{1 - |\nabla u|^2}} \right) = 0 \quad [10]$$

N maximizes area with respect to compactly supported variations, and hence is called a maximal surface. As in the case of the minimal surface equation, eqn [10] and more generally the

Lorentzian prescribed mean curvature equation, is quasilinear elliptic, but it is not uniformly elliptic, which makes the regularity theory more subtle.

A Bernstein principle analogous to the one for the minimal surface equation holds for the maximal surface equation [10]. Suppose that u is a solution to [10] which is defined on all of \mathbb{R}^n . Then u is an affine function (Cheng and Yau 1976). An important tool used in the proof is a Bochner type identity, originally due to Calabi, for the norm of the second fundamental form. For a hypersurface in a flat ambient space, the Codazzi equation states $\nabla_i A_{jk} - \nabla_j A_{ik} = 0$. This gives the identity

$$\Delta A_{ij} = \nabla_i \nabla_j H + A_{km} R_{i j}^m + A_{mi} \text{Ric}_j^m \quad [11]$$

The curvature terms can be rewritten in terms of A_{ij} if the ambient space is flat. Using [11] to compute $\Delta |A|^2$ gives an expression which is quadratic in ∇A , and fourth order in $|A|$, and which allows one to perform maximum principle estimates on $|A|$. Generalizations of this technique for hypersurfaces in general ambient spaces play an important role in the proof of regularity of minimal surfaces, and in the proof of existence for Jang's equation as well as in the analysis of the mean curvature flow used to prove existence of round spheres. The generalization of eqn [11] is known as a Simons identity.

For the case of maximal hypersurfaces of Minkowski space, it follows from further maximum principle estimates that a maximal hypersurface of Minkowski space is convex, in particular, it has nonpositive Ricci curvature. Generalizations of this technique allow one to analyze entire constant mean curvature hypersurfaces of Minkowski space.

Consider a globally hyperbolic Lorentzian manifold (V, γ) . A C^0 hypersurface is said to be weakly spacelike if timelike curves intersect it in at most one point. Call a codimension-2 submanifold $\Gamma \subset V$ a weakly spacelike boundary if it bounds a weakly spacelike hypersurface N_0 .

Theorem 5 (Existence for Plateau problem for maximal surfaces (Bartnik 1988)). *Let V be a globally hyperbolic spacetime and assume that the causal structure of V is such that the domain of dependence of any compact domain in V is compact. Given a weakly spacelike boundary Γ in V , there is a weakly spacelike maximal hypersurface N with Γ as its boundary. N is smooth except possibly on null geodesics connecting points of Γ .*

Here, maximal hypersurface is understood in a weak sense, referring to stationarity with respect to variations. Due to the nonuniform ellipticity for the maximal surface equation, the interior regularity

which holds for minimal surfaces fails to hold in general for the maximal surface equation.

A time-oriented spacetime is said to have a crushing singularity to the past (future) if there is a sequence Σ_n of Cauchy surfaces so that the mean curvature function H_n of Σ_n diverges uniformly to $-\infty(\infty)$.

Theorem 6 (Gerhardt 1983). *Suppose that (V, γ) is globally hyperbolic with compact Cauchy surfaces and satisfies the SEC. Then if (V, γ) has crushing singularities to the past and future it is globally foliated by constant mean curvature hypersurfaces. The mean curvature τ of these Cauchy surfaces is a global time function.*

The proof involves an application of results from geometric measure theory to an action \mathcal{E} of the form discussed earlier. A barrier argument is used to control the maximizers. Bartnik (1984, theorem 4.1) gave a direct proof of existence of a constant mean curvature (CMC) hypersurface, given barriers. If the spacetime (V, γ) is symmetric, so that a compact Lie group acts on V by isometries, then CMC hypersurfaces in V inherit the symmetry. Theorem 6 gives a condition under which a spacetime is globally foliated by CMC hypersurfaces. In general, if the SEC holds in a spatially compact spacetime, then for each $\tau \neq 0$, there is at most one constant mean curvature Cauchy surface with mean curvature τ . In case V is vacuum, $\text{Ric}_V = 0$, and $3 + 1$ dimensional, then each point $x \in V$ is on at most one hypersurface of constant mean curvature unless V is flat and splits as a metric product.

There are vacuum spacetimes with compact Cauchy surface which contain no CMC hypersurface (Chrusi el *et al.* 2004). The proof is carried out by constructing Cauchy data, using a gluing argument, on the connected sum of two tori, such that the resulting Cauchy data set (M, g_{ij}, K_{ij}) has an involution which reverses the sign of K_{ij} . The involution extends to the maximal vacuum development V of the Cauchy data set. Existence of a CMC surface in V gives, in view of the involution, barriers which allow one to construct a maximal Cauchy surface homeomorphic to M . This leads to a contradiction, since the connected sum of two tori does not carry a metric of positive scalar curvature, and therefore, in view of the constraint equations, cannot be imbedded as a maximal Cauchy surface in a vacuum spacetime. The maximal vacuum development V is causally geodesically incomplete. However, in view of the existence proof for CMC Cauchy surfaces (cf. Theorem 6), these spacetimes cannot have a crushing singularity. It would be interesting to settle the open question whether there are stable examples of this type.

In the case of a spacetime V which has an expanding end, one does not expect in general that

the spacetime is globally foliated by CMC hypersurfaces even if V is vacuum and contains a CMC Cauchy surface. This expectation is based on the phenomenon known as the collapse of the lapse; for example, the Schwarzschild spacetime does not contain a global foliation by maximal Cauchy surfaces (Beig and Murchadha 1998). However, no counterexample is known in the spatially compact case. In spite of these caveats, many examples of spacetimes with global CMC foliations are known, and the CMC condition, or more generally prescribed mean curvature, is an important gauge condition for general relativity.

Some examples of situations where global constant or prescribed mean curvature foliations are known to exist in vacuum or with some types of matter are spatially homogeneous spacetimes, and spacetimes with two commuting Killing fields. Small data global existence for the Einstein equations with CMC time gauge have been proved for spacetimes with one Killing field, with Cauchy surface a circle bundle over a surface of genus > 1 , by Choquet-Bruhat and Moncrief. Further, for $(3 + 1)$ -dimensional spacetimes with Cauchy surface admitting a hyperbolic metric, small data global existence in the expanding direction has been proved by Andersson and Moncrief. See Andersson (2004) and Rendall (2002) for surveys on the Cauchy problem in general relativity.

Null Hypersurfaces

Consider an asymptotically flat spacetime containing a black hole, that is, a region B such that future causal curves starting in B cannot reach observers at infinity. The boundary of the trapped region is called the event horizon \mathcal{H} . This is a null hypersurface, which under reasonable conditions on causality has null generators which are complete to the future. Due to the completeness, assuming that \mathcal{H} is smooth, one can use the Raychaudhuri equation [7] to show that the null expansion θ_+ of a spatial cross section of \mathcal{H} must satisfy $\theta_+ \geq 0$, and hence that the area of cross sections of \mathcal{H} grows monotonously to the future. A related statement is that null generators can enter \mathcal{H} but may not leave it. This was first proved by Hawking for the case of smooth horizons, using essentially the Raychaudhuri equation. In general \mathcal{H} can fail to be smooth. However, from the definition of \mathcal{H} as the boundary of the trapped region it follows that it has support hypersurfaces, which are past light cones. This property allows one to prove that \mathcal{H} is Lipschitz and hence smooth almost everywhere. At smooth points of \mathcal{H} , the calculations in the proof of

Hawking apply, and the monotonicity of the area of cross sections follows.

Theorem 7 (Area theorem (Chrusciel *et al.* 2001)). *Let \mathcal{H} be a black hole event horizon in a smooth spacetime (M, g) . Suppose that the generators are future complete and the NEC holds on \mathcal{H} . Let $S_a, a = 1, 2$, be two spacelike cross sections of \mathcal{H} and suppose that S_2 is to the future of S_1 . Then $A(S_2) \geq A(S_1)$.*

The eikonal equation $\nabla^\alpha u \nabla_\alpha u = 0$ plays a central role in geometric optics. Level sets of a solution u are null hypersurfaces which correspond to wave fronts. Much of the recent progress on rough solutions to the Cauchy problem for quasilinear wave equations is based on understanding the influence of the geometry of these wave fronts on the evolution of high-frequency modes ‘in the background spacetime. In this analysis many objects familiar from general relativity, such as the structure equations for null hypersurfaces, the Raychaudhuri equation, and the Bianchi identities play an important role, together with novel techniques of geometric analysis used to control the geometry of cross sections of the wave fronts and to estimate the connection coefficients in a rough spacetime geometry. These techniques show great promise and can be expected to have a significant impact on our understanding of the Einstein equations and general relativity.

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See also: Computational Methods in General Relativity: The Theory; Einstein Equations: Initial Value Formulation; Einstein's Equations with Matter; Geometric Flows and the Penrose Inequality; Hamiltonian Reduction of Einstein's Equations; Holomorphic Dynamics; Lorentzian Geometry; Minimal Submanifolds; Mirror Symmetry: A Geometric Survey; Spacetime Topology, Causal Structure and Singularities; Stability of Minkowski Space.

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Geometric Flows and the Penrose Inequality

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Introduction

In a paper, R Penrose (1973) made a physical argument that the total mass of a spacetime which contains black holes with event horizons of total area A should be at least $\sqrt{A/16\pi}$. An important special case of this physical statement translates into a very beautiful mathematical inequality in Riemannian geometry known as the Riemannian Penrose inequality. The Riemannian Penrose inequality was first proved by Huisken and Ilmanen (1997) for a single black hole and then by the author in 1999 for any number of black holes. The two approaches use two different geometric flow techniques. The most general version of the Penrose inequality is still open.

A natural interpretation of the Penrose inequality is that the mass contributed by a collection of black holes is (at least) $\sqrt{A/16\pi}$. More generally, the question "How much matter is in a given region of a spacetime?" is still very much an open problem. (Christodoulou and Yau 1988). In this paper, we will discuss some of the qualitative aspects of mass in general relativity, look at examples which are informative, and describe the two very geometric proofs of the Riemannian Penrose inequality.

Total Mass in General Relativity

Two notions of mass which are well understood in general relativity are local energy density at a point and the total mass of an asymptotically flat spacetime. However, defining the mass of a region larger than a point but smaller than the entire universe is not very well understood at all.

Suppose (M^3, g) is a Riemannian 3-manifold isometrically embedded in a $(3+1)$ -dimensional Lorentzian spacetime N^4 . Suppose that M^3 has zero-second fundamental form in the spacetime. This is a simplifying assumption which allows us to think of (M^3, g) as a " $t=0$ " slice of the spacetime. (Recall that the second fundamental form is a measure of how much M^3 curves inside N^4 . M^3 is also sometimes called "totally geodesic" since geodesics of N^4 which are tangent to M^3 at a point stay inside M^3 forever.) The Penrose inequality (which allows for M^3 to have general second fundamental form) is known as the

Riemannian Penrose inequality when the second fundamental form is set to zero.

We also want to only consider (M^3, g) that are asymptotically flat at infinity, which means that for some compact set K , the "end" $M^3 \setminus K$ is diffeomorphic to $\mathbb{R}^3 \setminus B_1(0)$, where the metric g is asymptotically approaching (with certain decay conditions) the standard flat metric δ_{ij} on \mathbb{R}^3 at infinity. The simplest example of an asymptotically flat manifold is $(\mathbb{R}^3, \delta_{ij})$ itself. Other good examples are the conformal metrics $(\mathbb{R}^3, u(x)^4 \delta_{ij})$, where $u(x)$ approaches a constant sufficiently rapidly at infinity. (Also, sometimes it is convenient to allow (M^3, g) to have multiple asymptotically flat ends, in which case each connected component of $M^3 \setminus K$ must have the property described above.) A qualitative picture of an asymptotically flat 3-manifold is shown in Figure 1.

The purpose of these assumptions on the asymptotic behavior of (M^3, g) at infinity is that they imply the existence of the limit

$$m = \frac{1}{16\pi} \lim_{\sigma \rightarrow \infty} \int_{S_\sigma} \sum_{i,j} (g_{ij,i} \nu_j - g_{ii,j} \nu_j) d\mu$$

where S_σ is the coordinate sphere of radius σ , ν is the unit normal to S_σ , and $d\mu$ is the area element of S_σ in the coordinate chart. The quantity m is called the "total mass" (or ADM mass) of (M^3, g) and does not depend on the choice of asymptotically flat coordinate chart.

The above equation is where many people would stop reading an article like this. But before you do, we will promise not to use this definition of the total mass in this paper. In fact, it turns out that total mass can be quite well understood with an example. Going back to the example $(\mathbb{R}^3, u(x)^4 \delta_{ij})$, if we suppose that $u(x) > 0$ has the asymptotics at infinity

$$u(x) = a + b/|x| + \mathcal{O}(1/|x|^2) \quad [1]$$

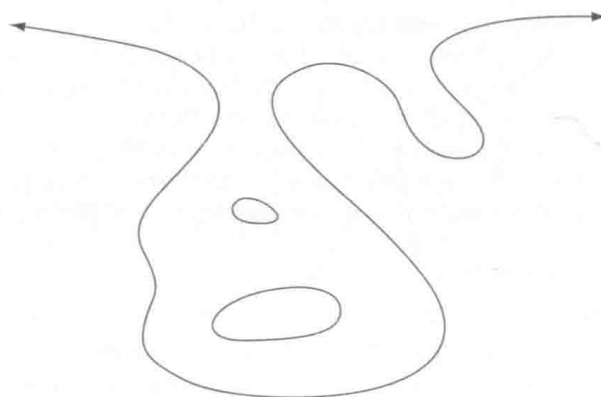


Figure 1 A qualitative picture of an asymptotically flat 3-manifold.

(and derivatives of the $\mathcal{O}(1/|x|^2)$ term are $\mathcal{O}(1/|x|^3)$), then the total mass of (M^3, g) is

$$m = 2ab \quad [2]$$

Furthermore, suppose (M^3, g) is any metric whose “end” is isometric to $(\mathbb{R}^3 \setminus K, u(x)^4 \delta_{ij})$, where $u(x)$ is harmonic in the coordinate chart of the end $(\mathbb{R}^3 \setminus K, \delta_{ij})$ and goes to a constant at infinity. Then expanding $u(x)$ in terms of spherical harmonics demonstrates that $u(x)$ satisfies condition [1]. We will call these Riemannian manifolds (M^3, g) “harmonically flat at infinity,” and we note that the total mass of these manifolds is also given by eqn [2].

A very nice lemma by Schoen and Yau is that, given any $\epsilon > 0$, it is always possible to perturb an asymptotically flat manifold to become harmonically flat at infinity such that the total mass changes less than ϵ and the metric changes less than ϵ pointwise, all while maintaining non-negative scalar curvature. Hence, it happens that to prove the theorems in this paper, we only need to consider harmonically flat manifolds! Thus, we can use eqn [2] as our definition of total mass. As an example, note that $(\mathbb{R}^3, \delta_{ij})$ has zero total mass. Also, note that, qualitatively, the total mass of an asymptotically flat or harmonically flat manifold is the $1/r$ rate at which the metric becomes flat at infinity.

The Phenomenon of Gravitational Attraction

What do the above definitions of total mass have to do with anything physical? That is, if the total mass is the $1/r$ rate at which the metric becomes flat at infinity, what does this have to do with our real-world intuitive idea of mass?

The answer to this question is very nice. Given a Schwarzschild spacetime metric

$$\left(\mathbb{R}^4, \left(1 + \frac{m}{2|x|} \right)^4 (dx_1^2 + dx_2^2 + dx_3^2) - \left(\frac{1 - m/2|x|}{1 + m/2|x|} \right)^2 dt^2 \right)$$

$|x| > m/2$, for example, note that the $t=0$ slice (which has zero-second fundamental form) is the spacelike Schwarzschild metric

$$\left(\mathbb{R}^3 \setminus B_{m/2}(0), \left(1 + \frac{m}{2|x|} \right)^4 \delta_{ij} \right)$$

(discussed more later). Note that according to eqn [2], the parameter m is in fact the total mass of this 3-manifold.

On the other hand, suppose we were to release a small test particle, initially at rest, a large distance r from the center of the Schwarzschild spacetime. If

this particle is not acted upon by external forces, then it should follow a geodesic in the spacetime. It turns out that with respect to the asymptotically flat coordinate chart, these geodesics “accelerate” towards the middle of the Schwarzschild metric proportional to m/r^2 (in the limit as r goes to infinity). Thus, our Newtonian notion of mass also suggests that the total mass of the spacetime is m .

Local Energy Density

Another quantification of mass which is well understood is local energy density. In fact, in this setting, the local energy density at each point is

$$\mu = \frac{1}{16\pi} R$$

where R is the scalar curvature of the 3-manifold (which has zero-second fundamental form in the spacetime) at each point. Note that $(\mathbb{R}^3, \delta_{ij})$ has zero energy density at each point as well as zero total mass. This is appropriate since $(\mathbb{R}^3, \delta_{ij})$ is in fact a “ $t=0$ ” slice of Minkowski spacetime, which represents a vacuum. Classically, physicists consider $\mu \geq 0$ to be a physical assumption. Hence, from this point on, we will not only assume that (M^3, g) is asymptotically flat, but also that it has non-negative scalar curvature,

$$R \geq 0$$

This notion of energy density also helps us understand total mass better. After all, we can take any asymptotically flat manifold and then change the metric to be perfectly flat outside a large compact set, thereby giving the new metric zero total mass. However, if we introduce the physical condition that both metrics have non-negative scalar curvature, then it is a beautiful theorem that this is in fact not possible, unless the original metric was already $(\mathbb{R}^3, \delta_{ij})$! (This theorem is actually a corollary to the positive mass theorem discussed below.) Thus, the curvature obstruction of having non-negative scalar curvature at each point is a very interesting condition.

Also, notice the indirect connection between the total mass and local energy density. At this point, there does not seem to be much of a connection at all. The total mass is the $1/r$ rate at which the metric becomes flat at infinity, and local energy density is the scalar curvature at each point. Furthermore, if a metric is changed in a compact set, local energy density is changed, but the total mass is unaffected.

The reason for this is that the total mass is “not” the integral of the local energy density over the manifold. In fact, this integral fails to take potential energy into account (which would be expected to

contribute a negative energy) as well as gravitational energy. Hence, it is not initially clear what we should expect the relationship between total mass and local energy density to be, so let us begin with an example.

Example Using Superharmonic Functions in \mathbb{R}^3

Once again, let us return to the $(\mathbb{R}^3, u(x)^4 \delta_{ij})$ example. The formula for the scalar curvature is

$$R = -8u(x)^{-5} \Delta u(x)$$

Hence, since the physical assumption of non-negative energy density implies non-negative scalar curvature, we see that $u(x) > 0$ must be superharmonic ($\Delta u \leq 0$). For simplicity, let us also assume that $u(x)$ is harmonic outside a bounded set so that we can expand $u(x)$ at infinity using spherical harmonics. Hence, $u(x)$ has the asymptotics of eqn [1]. By the maximum principle, it follows that the minimum value for $u(x)$ must be a , referring to eqn [1]. Hence, $b \geq 0$, which implies that $m \geq 0$! Thus, we see that the assumption of non-negative energy density at each point of $(\mathbb{R}^3, u(x)^4 \delta_{ij})$ implies that the total mass is also non-negative, which is what one would hope.

The Positive Mass Theorem

Why would one hope this? What would be the difference if the total mass were negative? This would mean that a gravitational system of positive energy density could collectively act as a net negative total mass. This phenomenon has not been observed experimentally, and so it is not a property that we would hope to find in general relativity.

More generally, suppose we have any asymptotically flat manifold with non-negative scalar curvature, is it true that the total mass is also non-negative? The answer is yes, and this fact is known as the positive mass theorem, first proved by Schoen and Yau (1979) using minimal surface techniques and then by Witten (1981) using spinors. In the zero-second fundamental form case, the positive mass theorem is known as the Riemannian positive mass theorem and is stated below.

Theorem 1 (Schoen, Yau). *Let (M^3, g) be any asymptotically flat, complete Riemannian manifold with non-negative scalar curvature. Then the total mass $m \geq 0$, with equality if and only if (M^3, g) is isometric to (\mathbb{R}^3, δ) .*

Gravitational Energy

The previous example neglects to illustrate some of the subtleties of the positive mass theorem. For example, it is easy to construct asymptotically flat

manifolds (M^3, g) (not conformal to \mathbb{R}^3) which have zero scalar curvature everywhere and yet have “nonzero” total mass. By the positive mass theorem, the mass of these manifolds is positive. Physically, this corresponds to a spacetime with zero energy density everywhere which still has positive total mass. From where did this mass come? How can a vacuum have positive total mass?

Physicists refer to this extra energy as gravitational energy. There is no known local definition of the energy density of a gravitational field, and presumably such a definition does not exist. The curious phenomenon, then, is that for some reason, gravitational energy always makes a non-negative contribution to the total mass of the system.

Black Holes

Another very interesting and natural phenomenon in general relativity is the existence of black holes. Instead of thinking of black holes as singularities in a spacetime, we will think of black holes in terms of their horizons. For example, suppose we are exploring the universe in a spacecraft capable of traveling at any speed less than the speed of light. If we are investigating a black hole, we would want to make sure that we don’t get too close and get trapped by the “gravitational forces” of the black hole. In fact, we could imagine a “sphere of no return” beyond which it is impossible to escape from the black hole. This is called the event horizon of a black hole.

However, one limitation of the notion of an event horizon is that it is very hard to determine its location. One way is to let daredevil spacecraft see how close they can get to the black hole and still escape from it eventually. The only problem with this approach (besides the cost in spacecraft) is that it is hard to know when to stop waiting for a daredevil spacecraft to return. Even if it has been 50 years, it could be that this particular daredevil was not trapped by the black hole but got so close that it will take it 1000 or more years to return. Thus, to define the location of an event horizon even mathematically, we need to know the entire evolution of the spacetime. Hence, event horizons can not be computed based only on the local geometry of the spacetime.

This problem is solved (at least for the mathematician) with the notion of apparent horizons of black holes. Given a surface in a spacetime, suppose that it emits an outward shell of light. If the surface area of this shell of light is decreasing everywhere on the surface, then this is called a trapped surface. The outermost boundary of these trapped surfaces is called the apparent horizon of the black hole. Apparent horizons can be computed based on their

local geometry, and an apparent horizon always implies the existence of an event horizon outside of it (Hawking and Ellis 1973).

Now let us return to the case we are considering in this paper where (M^3, g) is a “ $t=0$ ” slice of a spacetime with zero-second fundamental form. Then it is a very nice geometric fact that apparent horizons of black holes intersected with M^3 correspond to the connected components of the outermost minimal surface Σ_0 of (M^3, g) .

All of the surfaces we are considering in this paper will be required to be smooth boundaries of open bounded regions, so that outermost is well defined with respect to a chosen end of the manifold. A minimal surface in (M^3, g) is a surface which is a critical point of the area function with respect to any smooth variation of the surface. The first variational calculation implies that minimal surfaces have zero mean curvature. The surface Σ_0 of (M^3, g) is defined as the boundary of the union of the open regions bounded by all of the minimal surfaces in (M^3, g) . It turns out that Σ_0 also has to be a minimal surface, so we call Σ_0 the “outermost minimal surface.” A qualitative sketch of an outermost minimal surface of a 3-manifold is shown in Figure 2.

We will also define a surface to be “(strictly) outer minimizing” if every surface which encloses it has (strictly) greater area. Note that outermost minimal surfaces are strictly outer minimizing. Also, we define a “horizon” in our context to be any minimal surface which is the boundary of a bounded open region.

It also follows from a stability argument (using the Gauss–Bonnet theorem interestingly) that each component of an outermost minimal surface (in a 3-manifold with non-negative scalar curvature) must have the topology of a sphere. Furthermore, there is a physical argument, based on Penrose (1973), which suggests that the mass contributed by the black holes (thought of as the connected components of Σ_0) should be defined to be $\sqrt{A_0/16\pi}$,

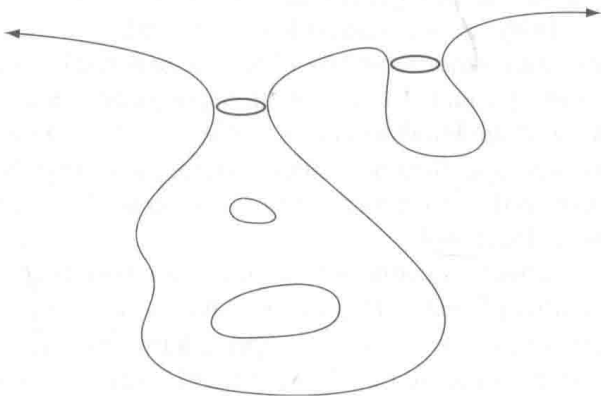


Figure 2 A qualitative sketch of an outermost minimal surface of a 3-manifold.

where A_0 is the area of Σ_0 . Hence, the physical argument that the total mass should be greater than or equal to the mass contributed by the black holes yields the following geometric statement.

The Riemannian Penrose Inequality Let (M^3, g) be a complete, smooth, 3-manifold with non-negative scalar curvature which is harmonically flat at infinity with total mass m and which has an outermost minimal surface Σ_0 of area A_0 . Then,

$$m \geq \sqrt{\frac{A_0}{16\pi}} \quad [3]$$

with equality if and only if (M^3, g) is isometric to the Schwarzschild metric

$$\left(\mathbb{R}^3 \setminus \{0\}, \left(1 + \frac{m}{2|x|} \right)^4 \delta_{ij} \right)$$

outside their respective outermost minimal surfaces.

The above statement has been proved by the present author, and Huisken and Ilmanen proved it when A_0 is defined instead to be the area of the largest connected component of Σ_0 . We will discuss both approaches in this paper, which are very different, although they both involve flowing surfaces and/or metrics.

We also clarify that the above statement is with respect to a chosen end of (M^3, g) , since both the total mass and the definition of outermost refer to a particular end. In fact, nothing very important is gained by considering manifolds with more than one end, since extra ends can always be compactified by connect summing them (around a neighborhood of infinity) with large spheres while still preserving non-negative scalar curvature, for example. Hence, we will typically consider manifolds with just one end. In the case that the manifold has multiple ends, we will require every surface (which could have multiple connected components) in this paper to enclose all of the ends of the manifold except the chosen end.

The Schwarzschild Metric

The Schwarzschild metric

$$\left(\mathbb{R}^3 \setminus \{0\}, \left(1 + \frac{m}{2|x|} \right)^4 \delta_{ij} \right)$$

referred to in the above statement of the Riemannian Penrose inequality, is a particularly important example to consider, and corresponds to a zero-second fundamental form, spacelike slice of the usual $(3+1)$ -dimensional Schwarzschild metric (which represents a spherically symmetric static black hole in vacuum). The three-dimensional

Schwarzschild metrics have total mass $m > 0$ and are characterized by being the only spherically symmetric, geodesically complete, zero scalar curvature 3-metrics, other than $(\mathbb{R}^3, \delta_{ij})$. They can also be embedded in four-dimensional Euclidean space (x, y, z, w) as the set of points satisfying

$$|(x, y, z)| = (w^2/8m) + 2m$$

which is a parabola rotated around an S^2 . This last picture allows us to see that the Schwarzschild metric, which has two ends, has a Z_2 symmetry which fixes the sphere with $w=0$ and $|(x, y, z)| = 2m$, which is clearly minimal. Furthermore, the area of this sphere is $4\pi(2m)^2$, giving equality in the Riemannian Penrose inequality.

A Brief History of the Problem

The Riemannian Penrose inequality has a rich history spanning nearly three decades and has motivated much interesting mathematics and physics. In 1973, R Penrose in effect conjectured an even more general version of inequality [3] using a very clever physical argument, which we will not have room to repeat here (Penrose 1973). His observation was that a counterexample to inequality [3] would yield Cauchy data for solving the Einstein equations, the solution to which would likely violate the cosmic censor conjecture (which says that singularities generically do not form in a spacetime unless they are inside a black hole).

Jang and Wald (1977), extending ideas of Geroch, gave a heuristic proof of inequality [3] by defining a flow of 2-surfaces in (M^3, g) in which the surfaces flow in the outward normal direction at a rate equal to the inverse of their mean curvatures at each point. The Hawking mass of a surface (which is supposed to estimate the total amount of energy inside the surface) is defined to be

$$m_{\text{Hawking}}(\Sigma) = \sqrt{\frac{|\Sigma|}{16\pi}} \left(1 - \frac{1}{16\pi} \int_{\Sigma} H^2 \right)$$

(where $|\Sigma|$ is the area of Σ and H is the mean curvature of Σ in (M^3, g)) and, amazingly, is nondecreasing under this “inverse mean curvature flow.” This is seen by the fact that under inverse mean curvature flow, it follows from the Gauss equation and the second variation formula that

$$\begin{aligned} \frac{d}{dt} m_{\text{Hawking}}(\Sigma) = & \sqrt{\frac{|\Sigma|}{16\pi}} \left[\frac{1}{2} + \frac{1}{16\pi} \int_{\Sigma} 2 \frac{|\nabla_{\Sigma} H|^2}{H^2} \right. \\ & \left. + R - 2K + \frac{1}{2}(\lambda_1 - \lambda_2)^2 \right] \end{aligned}$$

when the flow is smooth, where R is the scalar curvature of (M^3, g) , K is the Gauss curvature of the surface Σ , and λ_1 and λ_2 are the eigenvalues of the second fundamental form of Σ , or principle curvatures. Hence,

$$R \geq 0$$

and

$$\int_{\Sigma} K \leq 4\pi \quad [4]$$

(which is true for any connected surface by the Gauss–Bonnet theorem) imply

$$\frac{d}{dt} m_{\text{Hawking}}(\Sigma) \geq 0 \quad [5]$$

Furthermore,

$$m_{\text{Hawking}}(\Sigma_0) = \sqrt{\frac{|\Sigma_0|}{16\pi}}$$

since Σ_0 is a minimal surface and has zero mean curvature. In addition, the Hawking mass of sufficiently round spheres at infinity in the asymptotically flat end of (M^3, g) approaches the total mass m . Hence, if inverse mean curvature flow beginning with Σ_0 eventually flows to sufficiently round spheres at infinity, inequality [3] follows from inequality [5].

As noted by Jang and Wald, this argument only works when inverse mean curvature flow exists and is smooth, which is generally not expected to be the case. In fact, it is not hard to construct manifolds which do not admit a smooth inverse mean curvature flow. The problem is that if the mean curvature of the evolving surface becomes zero or is negative, it is not clear how to define the flow.

For 20 years, this heuristic argument lay dormant until the work of Huisken and Ilmanen in 1997. With a very clever new approach, Huisken and Ilmanen discovered how to reformulate inverse mean curvature flow using an energy minimization principle in such a way that the new generalized inverse mean curvature flow always exists. The added twist is that the surface sometimes jumps outward. However, when the flow is smooth, it equals the original inverse mean curvature flow, and the Hawking mass is still monotone. Hence, as will be described in the next section, their new flow produced the first complete proof of inequality [3] for a single black hole.

Coincidentally, the author found another proof of inequality [3], submitted in 1999, which works for any number of black holes. The approach involves flowing the original metric to a Schwarzschild metric (outside the horizon) in such a way that the area of the outermost minimal surface does not change and the

total mass is nonincreasing. Then, since the Schwarzschild metric gives equality in inequality [3], the inequality follows for the original metric.

Fortunately, the flow of metrics which is defined is relatively simple, and in fact stays inside the conformal class of the original metric. The outermost minimal surface flows outwards in this conformal flow of metrics, and encloses any compact set (and hence all of the topology of the original metric) in a finite amount of time. Furthermore, this conformal flow of metrics preserves non-negative scalar curvature. We will describe this approach later in the paper.

Other contributions on the Penrose conjecture have also been made by Herzlich using the Dirac operator which Witten used to prove the positive mass theorem, by Gibbons in the special case of collapsing shells, by Tod, by Bartnik for quasi-spherical metrics, and by the present author using isoperimetric surfaces. There is also some interesting work of Ludvigsen and Vickers using spinors and Bergqvist, both concerning the Penrose inequality for null slices of a spacetime.

Inverse Mean Curvature Flow

Geometrically, Huisken and Ilmanen's idea can be described as follows. Let $\Sigma(t)$ be the surface resulting from inverse mean curvature flow for time t beginning with the minimal surface Σ_0 . Define $\bar{\Sigma}(t)$ to be the outermost minimal area enclosure of $\Sigma(t)$. Typically, $\Sigma(t) = \bar{\Sigma}(t)$ in the flow, but in the case that the two surfaces are not equal, immediately replace $\Sigma(t)$ with $\bar{\Sigma}(t)$ and then continue flowing by inverse mean curvature.

An immediate consequence of this modified flow is that the mean curvature of $\bar{\Sigma}(t)$ is always non-negative by the first variation formula, since otherwise $\bar{\Sigma}(t)$ would be enclosed by a surface with less area. This is because if we flow a surface Σ in the outward direction with speed η , the first variation of the area is $\int_{\Sigma} H\eta$, where H is the mean curvature of Σ .

Furthermore, by stability, it follows that in the regions where $\bar{\Sigma}(t)$ has zero mean curvature, it is always possible to flow the surface out slightly to have positive mean curvature, allowing inverse mean curvature flow to be defined, at least heuristically at this point.

Furthermore, the Hawking mass is still monotone under this new modified flow. Notice that when $\Sigma(t)$ jumps outwards to $\bar{\Sigma}(t)$,

$$\int_{\bar{\Sigma}(t)} H^2 \leq \int_{\Sigma(t)} H^2$$

since $\bar{\Sigma}(t)$ has zero mean curvature where the two surfaces do not touch. Furthermore,

$$|\bar{\Sigma}(t)| = |\Sigma(t)|$$

since (this is a neat argument) $|\bar{\Sigma}(t)| \leq |\Sigma(t)|$ (since $\bar{\Sigma}(t)$ is a minimal area enclosure of $\Sigma(t)$) and we cannot have $|\bar{\Sigma}(t)| < |\Sigma(t)|$ since $\Sigma(t)$ would have jumped outwards at some earlier time. This is only a heuristic argument, but we can then see that the Hawking mass is nondecreasing during a jump by the above two equations.

This new flow can be rigorously defined, always exists, and the Hawking mass is monotone. Huisken and Ilmanen define $\Sigma(t)$ to be the level sets of a scalar valued function $u(x)$ defined on (M^3, g) such that $u(x) = 0$ on the original surface Σ_0 and satisfies

$$\operatorname{div} \left(\frac{\nabla u}{|\nabla u|} \right) = |\nabla u| \quad [6]$$

in an appropriate weak sense. Since the left-hand side of the above equation is the mean curvature of the level sets of $u(x)$ and the right-hand side is the reciprocal of the flow rate, the above equation implies inverse mean curvature flow for the level sets of $u(x)$ when $|\nabla u(x)| \neq 0$.

Huisken and Ilmanen use an energy minimization principle to define weak solutions to eqn [6]. Equation [6] is said to be weakly satisfied in Ω by the locally Lipschitz function u if for all locally Lipschitz v with $\{v \neq u\} \subset\subset \Omega$,

$$J_u(u) \leq J_u(v)$$

where

$$J_u(v) := \int_{\Omega} |\nabla v| + v|\nabla u|$$

It can then be seen that the Euler-Lagrange equation of the above energy functional yields eqn [6].

In order to prove that a solution u exists to the above two equations, Huisken and Ilmanen regularize the degenerate elliptic equation 6 to the elliptic equation

$$\operatorname{div} \left(\frac{\nabla u}{\sqrt{|\nabla u|^2 + \epsilon^2}} \right) = \sqrt{|\nabla u|^2 + \epsilon^2}$$

Solutions to the above equation are then shown to exist using the existence of a subsolution, and then taking the limit as ϵ goes to zero yields a weak solution to eqn [6]. There are many details which we are skipping here, but these are the main ideas.

As it turns out, weak solutions $u(x)$ to eqn [6] often have flat regions where $u(x)$ equals a constant. Hence, the level sets $\Sigma(t)$ of $u(x)$ will be

discontinuous in t in this case, which corresponds to the “jumping out” phenomenon referred to at the beginning of this section.

We also note that since the Hawking mass of the level sets of $u(x)$ is monotone, this inverse mean curvature flow technique not only proves the Riemannian Penrose inequality, but also gives a new proof of the positive mass theorem in dimension 3. This is seen by letting the initial surface be a very small, round sphere (which will have approximately zero Hawking mass) and then flowing by inverse mean curvature, thereby proving $m \geq 0$.

The Huisken and Ilmanen inverse mean curvature flow also seems ideally suited for proving Penrose inequalities for 3-manifolds which have $R \geq -6$ and which are asymptotically hyperbolic. This situation occurs if (M^3, g) is chosen to be a constant mean curvature slice of the spacetime or if the spacetime is defined to solve the Einstein equation with nonzero cosmological constant. In these cases, there exists a modified Hawking mass which is monotone under inverse mean curvature flow which is the usual Hawking mass plus $4(|\Sigma|/16\pi)^{3/2}$. However, because the monotonicity of the Hawking mass relies on the Gauss–Bonnet theorem, these arguments do not work in higher dimensions, at least so far. Also, because of the need for eqn [4], inverse mean curvature flow only proves the Riemannian Penrose inequality for a single black hole. In the next section, we present a technique which proves the Riemannian Penrose inequality for any number of black holes, and which can likely be generalized to higher dimensions.

The Conformal Flow of Metrics

Given any initial Riemannian manifold (M^3, g_0) which has non-negative scalar curvature and which is harmonically flat at infinity, we will define a continuous, one-parameter family of metrics (M^3, g_t) , $0 \leq t < \infty$. This family of metrics will converge to a three-dimensional Schwarzschild metric and will have other special properties which will allow us to prove the Riemannian Penrose inequality for the original metric (M^3, g_0) .

In particular, let Σ_0 be the outermost minimal surface of (M^3, g_0) with area A_0 . Then, we will also define a family of surfaces $\Sigma(t)$ with $\Sigma(0) = \Sigma_0$ such that $\Sigma(t)$ is minimal in (M^3, g_t) . This is natural since as the metric g_t changes, we expect that the location of the horizon $\Sigma(t)$ will also change. Then, the interesting quantities to keep track of in this flow are $A(t)$, the total area of the horizon $\Sigma(t)$ in (M^3, g_t) , and $m(t)$, the total mass of (M^3, g_t) in the chosen end.

In addition to all of the metrics g_t having non-negative scalar curvature, we will also have the very nice properties that

$$\begin{aligned} A'(t) &= 0 \\ m'(t) &\leq 0 \end{aligned}$$

for all $t \geq 0$. Then, since (M^3, g_t) converges to a Schwarzschild metric (in an appropriate sense) which gives equality in the Riemannian Penrose inequality as described in the introduction,

$$m(0) \geq m(\infty) = \sqrt{\frac{A(\infty)}{16\pi}} = \sqrt{\frac{A(0)}{16\pi}} \quad [7]$$

which proves the Riemannian Penrose inequality for the original metric (M^3, g_0) . The hard part, then, is to find a flow of metrics which preserves non-negative scalar curvature and the area of the horizon, decreases total mass, and converges to a Schwarzschild metric as t goes to infinity.

The Definition of the Flow

In fact, the metrics g_t will all be conformal to g_0 . This conformal flow of metrics can be thought of as the solution to a first-order ODE in t defined by eqns [8]–[11]. Let

$$g_t = u_t(x)^4 g_0 \quad [8]$$

and $u_0(x) \equiv 1$. Given the metric g_t , define

$$\begin{aligned} \Sigma(t) &= \text{the outermost minimal area} \\ &\quad \text{enclosure of } \Sigma_0 \text{ in } (M^3, g_t) \end{aligned} \quad [9]$$

where Σ_0 is the original outer minimizing horizon in (M^3, g_0) . In the cases in which we are interested, $\Sigma(t)$ will not touch Σ_0 , from which it follows that $\Sigma(t)$ is actually a strictly outer minimizing horizon of (M^3, g_t) . Then given the horizon $\Sigma(t)$, define $v_t(x)$ such that

$$\begin{cases} \Delta_{g_0} v_t(x) \equiv 0 & \text{outside } \Sigma(t) \\ v_t(x) = 0 & \text{on } \Sigma(t) \\ \lim_{x \rightarrow \infty} v_t(x) = -e^{-t} \end{cases} \quad [10]$$

and $v_t(x) \equiv 0$ inside $\Sigma(t)$. Finally, given $v_t(x)$, define

$$u_t(x) = 1 + \int_0^t v_s(x) \, ds \quad [11]$$

so that $u_t(x)$ is continuous in t and has $u_0(x) \equiv 1$.

Note that eqn [11] implies that the first-order rate of change of $u_t(x)$ is given by $v_t(x)$. Hence, the first-order rate of change of g_t is a function of itself, g_0 , and $v_t(x)$ which is a function of g_0 , t , and $\Sigma(t)$ which is in turn a function of g_t and Σ_0 . Thus, the first-order rate of change of g_t is a function of t , g_t , g_0 , and Σ_0 .

Theorem 2 Taken together, eqns [8]–[11] define a first-order ODE in t for $u_t(x)$ which has a solution which is Lipschitz in the t variable, C^1 in the x variable everywhere, and smooth in the x variable outside $\Sigma(t)$. Furthermore, $\Sigma(t)$ is a smooth, strictly outer minimizing horizon in (M^3, g_t) for all $t \geq 0$, and $\Sigma(t_2)$ encloses but does not touch $\Sigma(t_1)$ for all $t_2 > t_1 \geq 0$.

Since $v_t(x)$ is a superharmonic function in (M^3, g_0) (harmonic everywhere except on $\Sigma(t)$, where it is weakly superharmonic), it follows that $u_t(x)$ is superharmonic as well. Thus, from eqn [11] we see that $\lim_{x \rightarrow \infty} u_t(x) = e^{-t}$ and consequently that $u_t(x) > 0$ for all t by the maximum principle. Then, since

$$R(g_t) = u_t(x)^{-5}(-8\Delta_{g_0} + R(g_0))u_t(x) \quad [12]$$

it follows that (M^3, g_t) is an asymptotically flat manifold with non-negative scalar curvature.

Even so, it still may not seem like g_t is particularly naturally defined since the rate of change of g_t appears to depend on t and the original metric g_0 in eqn [10]. We would prefer a flow where the rate of change of g_t can be defined purely as a function of g_t (and Σ_0 perhaps), and interestingly enough this actually does turn out to be the case! The present author has proved this very important fact and defined a new equivalence class of metrics called the harmonic conformal class. Then, once we decide to find a flow of metrics which stays inside the harmonic conformal class of the original metric (outside the horizon) and keeps the area of the horizon $\Sigma(t)$ constant, then we are basically forced to choose the particular conformal flow of metrics defined above.

Theorem 3 The function $A(t)$ is constant in t and $m(t)$ is nonincreasing in t , for all $t \geq 0$.

The fact that $A'(t) = 0$ follows from the fact that to first order the metric is not changing on $\Sigma(t)$ (since $v_t(x) = 0$ there) and from the fact that to first order the area of $\Sigma(t)$ does not change as it moves outward since $\Sigma(t)$ is a critical point for area in (M^3, g_t) . Hence, the interesting part of Theorem 3 is proving that $m'(t) \leq 0$. Curiously, this follows from a nice trick using the Riemannian positive mass theorem, which we describe later.

Another important aspect of this conformal flow of the metric is that outside the horizon $\Sigma(t)$, the manifold (M^3, g_t) becomes more and more spherically symmetric and “approaches” a Schwarzschild manifold $(\mathbb{R}^3 \setminus \{0\}, s)$ in the limit as t goes to ∞ . More precisely,

Theorem 4 For sufficiently large t , there exists a diffeomorphism ϕ_t between (M^3, g_t) outside the horizon $\Sigma(t)$ and a fixed Schwarzschild manifold

$(\mathbb{R}^3 \setminus \{0\}, s)$ outside its horizon. Furthermore, for all $\epsilon > 0$, there exists a T such that for all $t > T$, the metrics g_t and $\phi_t^*(s)$ (when determining the lengths of unit vectors of (M^3, g_t)) are within ϵ of each other and the total masses of the 2-manifolds are within ϵ of each other. Hence,

$$\lim_{t \rightarrow \infty} \frac{m(t)}{\sqrt{A(t)}} = \sqrt{\frac{1}{16\pi}}$$

Theorem 4 is not that surprising really although a careful proof is reasonably long. However, if one is willing to believe that the flow of metrics converges to a spherically symmetric metric outside the horizon, then Theorem 4 follows from two facts. The first fact is that the scalar curvature of (M^3, g_t) eventually becomes identically zero outside the horizon $\Sigma(t)$ (assuming (M^3, g_0) is harmonically flat). This follows from the facts that $\Sigma(t)$ encloses any compact set in a finite amount of time, that harmonically flat manifolds have zero scalar curvature outside a compact set, that $u_t(x)$ is harmonic outside $\Sigma(t)$, and eqn [12]. The second fact is that the Schwarzschild metrics are the only complete, spherically symmetric 3-manifolds with zero scalar curvature (except for the flat metric on \mathbb{R}^3).

The Riemannian Penrose inequality, inequality [3], then follows from eqn [7] using Theorems 2–4, for harmonically flat manifolds. Since asymptotically flat manifolds can be approximated arbitrarily well by harmonically flat manifolds while changing the relevant quantities arbitrarily little, the asymptotically flat case also follows. Finally, the case of equality of the Penrose inequality follows from a more careful analysis of these same arguments.

Qualitative Discussion

Figures 3 and 4 are meant to help illustrate some of the properties of the conformal flow of the metric. Figure 3 is the original metric which has a strictly outer minimizing horizon Σ_0 . As t increases, $\Sigma(t)$ moves outwards, but never inwards. In Figure 4, we can observe one of the consequences of the fact that $A(t) = A_0$ is constant in t . Since the metric is not changing inside $\Sigma(t)$, all of the horizons $\Sigma(s)$, $0 \leq s \leq t$

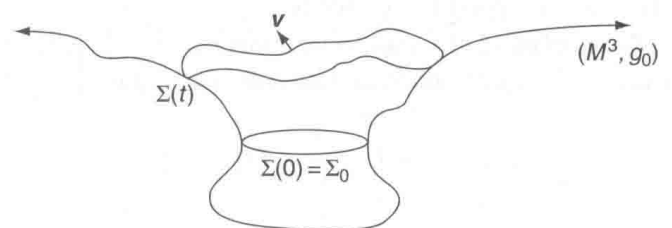


Figure 3 Original metric having a strictly outer minimizing horizon Σ_0 .

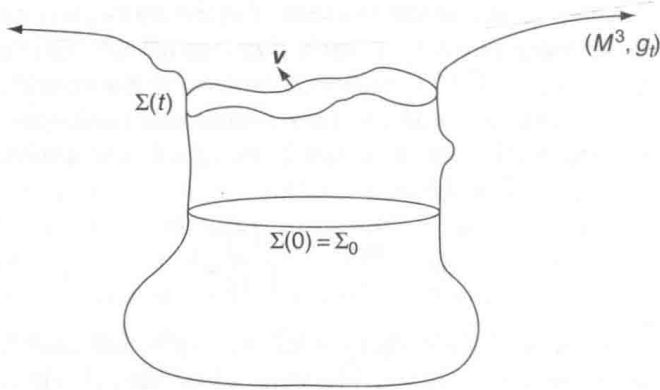


Figure 4 Metric after time t .

have area A_0 in (M^3, g_t) . Hence, inside $\Sigma(t)$, the manifold (M^3, g_t) becomes cylinder-like in the sense that it is laminated (i.e., foliated but with some gaps allowed) by all of the previous horizons which all have the same area A_0 with respect to the metric g_t .

Now let us suppose that the original horizon Σ_0 of (M^3, g) had two components, for example. Then each of the components of the horizon will move outwards as t increases, and at some point before they touch they will suddenly jump outwards to form a horizon with a single component enclosing the previous horizon with two components. Even horizons with only one component will sometimes jump outwards, but no more than a countable number of times. It is interesting that this phenomenon of surfaces jumping is also found in the Huisken–Ilmanen approach to the Penrose conjecture using their generalized $1/H$ flow.

Proof that $m'(t) \leq 0$

The most surprising aspect of the flow defined earlier is that $m'(t) \leq 0$. As mentioned in that section, this important fact follows from a nice trick using the Riemannian positive mass theorem.

The first step is to realize that while the rate of change of g_t appears to depend on t and g_0 , this is in fact an illusion. As described in detail by Bray, the rate of change of g_t can be described purely in terms of g_t (and Σ_0). It is also true that the rate of change of g_t depends only on g_t and $\Sigma(t)$. Hence, there is no special value of t , so proving $m'(t) \leq 0$ is equivalent to proving $m'(0) \leq 0$. Thus, without loss of generality, we take $t = 0$ for convenience.

Now expand the harmonic function $v_0(x)$, defined in eqn [10], using spherical harmonics at infinity, to get

$$v_0(x) = -1 + \frac{c}{|x|} + \mathcal{O}\left(\frac{1}{|x|^2}\right) \quad [13]$$

for some constant c . Since the rate of change of the metric g_t at $t = 0$ is given by $v_0(x)$ and since the total

mass $m(t)$ depends on the $1/r$ rate at which the metric g_t becomes flat at infinity (see eqn [2]), it is not surprising that direct calculation gives us that

$$m'(0) = 2(c - m(0))$$

Hence, to show that $m'(0) \leq 0$, we need to show that

$$c \leq m(0) \quad [14]$$

In fact, counterexamples to eqn [14] can be found if we remove either of the requirements that $\Sigma(0)$ (which is used in the definition of $v_0(x)$) be a minimal surface or that (M^3, g_0) have non-negative scalar curvature. Hence, we quickly see that eqn [14] is a fairly deep conjecture which says something quite interesting about manifold with non-negative scalar curvature. Well, the Riemannian positive mass theorem is also a deep conjecture which says something quite interesting about manifolds with non-negative scalar curvature. Hence, it is natural to try to use the Riemannian positive mass theorem to prove eqn [14].

Thus, we want to create a manifold whose total mass depends on c from eqn [13]. The idea is to use a reflection trick similar to one used by Bunting and Masood-ul-Alam (1987) for another purpose. First, remove the region of M^3 inside $\Sigma(0)$ and then reflect the remainder of (M^3, g_0) through $\Sigma(0)$. Define the resulting Riemannian manifold to be (\bar{M}^3, \bar{g}_0) which has two asymptotically flat ends since (M^3, g_0) has exactly one asymptotically flat end not contained by $\Sigma(0)$. Note that (\bar{M}^3, \bar{g}_0) has non-negative scalar curvature everywhere except on $\Sigma(0)$ where the metric has corners. In fact, the fact that $\Sigma(0)$ has zero mean curvature (since it is a minimal surface) implies that (\bar{M}^3, \bar{g}_0) has “distributional” non-negative scalar curvature everywhere, even on $\Sigma(0)$. This notion is made rigorous by Bray. Thus, we have used the fact that $\Sigma(0)$ is minimal in a critical way.

Recall from eqn [10] that $v_0(x)$ was defined to be the harmonic function equal to zero on $\Sigma(0)$ which goes to -1 at infinity. We want to reflect $v_0(x)$ to be defined on all of (\bar{M}^3, \bar{g}_0) . The trick here is to define $v_0(x)$ on (\bar{M}^3, \bar{g}_0) to be the harmonic function which goes to -1 at infinity in the original end and goes to 1 at infinity in the reflect end. By symmetry, $v_0(x)$ equals 0 on $\Sigma(0)$ and so agrees with its original definition on (M^3, g_0) .

The next step is to compactify one end of (\bar{M}^3, \bar{g}_0) . By the maximum principle, we know that $v_0(x) > -1$ and $c > 0$, so the new Riemannian manifold $(\bar{M}^3, (v_0(x) + 1)^4 \bar{g}_0)$ does the job quite nicely and compactifies the original end to a point. In fact, the compactified point at infinity and the metric there

can be filled in smoothly (using the fact that (M^3, g_0) is harmonically flat). It then follows from eqn [12] that this new compactified manifold has non-negative scalar curvature since $v_0(x) + 1$ is harmonic.

The last step is simply to apply the Riemannian positive mass theorem to $(\bar{M}^3, (v_0(x) + 1)^4 \bar{g}_0)$. It is not surprising that the total mass $\tilde{m}(0)$ of this manifold involves c , but it is quite lucky that direct calculation yields

$$\tilde{m}(0) = -4(c - m(0))$$

which must be positive by the Riemannian positive mass theorem. Thus, we have that

$$m'(0) = 2(c - m(0)) = -\frac{1}{2}\tilde{m}(0) \leq 0$$

Open Questions and Applications

Now that the Riemannian Penrose conjecture has been proved, what are the next interesting directions? What applications can be found? Is this subject only of physical interest, or are there possibly broader applications to other problems in mathematics?

Clearly, the most natural open problem is to find a way to prove the general Penrose inequality in which M^3 is allowed to have any second fundamental form in the spacetime. There is good reason to think that this may follow from the Riemannian Penrose inequality, although this is a bit delicate. On the other hand, the general positive mass theorem followed from the Riemannian positive mass theorem as was originally shown by Schoen and Yau using an idea due to Jang. For physicists, this problem is definitely a top priority since most spacetimes do not even admit zero-second fundamental form spacelike slices.

Another interesting question is to ask these same questions in higher dimensions. The author is currently working on a paper to prove the Riemannian Penrose inequality in dimensions < 8 . Dimension 8 and higher are harder because of the surprising fact that minimal hypersurfaces (and hence apparent horizons of black holes) can have codimension 7 singularities (points where the hypersurface is not smooth). This curious technicality is also the reason that the positive mass conjecture is still open in dimensions 8 and higher for manifolds which are not spin.

Naturally, it is harder to tell what the applications of these techniques might be to other problems, but already there have been some. One application is to the famous Yamabe problem: given a compact 3-manifold M^3 , define $E(g) = \int_{M^3} R_g dV_g$ where g is scaled so that the total volume of (M^3, g) is 1, R_g is the scalar curvature at each point, and dV_g is the volume form. An idea due to Yamabe was to try to

construct canonical metrics on M^3 by finding critical points of this energy functional on the space of metrics. Define $C(g)$ to be the infimum of $E(\bar{g})$ over all metrics \bar{g} conformal to g . Then the (topological) Yamabe invariant of M^3 , denoted here as $Y(M^3)$, is defined to be the supremum of $C(g)$ over all metrics g . $Y(S^3) = 6 \cdot (2\pi^2)^{2/3} \equiv Y_1$ is known to be the largest possible value for Yamabe invariants of 3-manifolds. It is also known that $Y(T^3) = 0$ and $Y(S^2 \times S^1) = Y_1 = Y(S^2 \tilde{\times} S^1)$, where $S^2 \tilde{\times} S^1$ is the nonorientable S^2 bundle over S^1 .

The author, working with Andre Neves on a problem suggested by Richard Schoen, recently was able to compute the Yamabe invariant of RP^3 using inverse mean curvature flow techniques and found that $Y(RP^3) = Y_1/2^{2/3} \equiv Y_2$. A corollary is $Y(RP^2 \times S^1) = Y_2$ as well. These techniques also yield the surprisingly strong result that the only prime 3-manifolds with Yamabe invariant larger than RP^3 are S^3 , $S^2 \times S^1$, and $S^2 \tilde{\times} S^1$. The Poincaré conjecture for 3-manifolds with Yamabe invariant greater than RP^3 is therefore a corollary. Furthermore, the problem of classifying 3-manifolds is known to reduce to the problem of classifying prime 3-manifolds. The Yamabe approach then would be to make a list of prime 3-manifolds ordered by Y . The first five prime 3-manifolds on this list are therefore S^3 , $S^2 \times S^1$, $S^2 \tilde{\times} S^1$, RP^3 , and $RP^2 \times S^1$.

Acknowledgments

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See also: Black Hole Mechanics; General Relativity: Experimental Tests; General Relativity: Overview; Geometric Analysis and General Relativity; Holomorphic Dynamics; Mirror Symmetry: A Geometric Survey; Spinors and Spin Coefficients; Stationary Black Holes.

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Geometric Measure Theory

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Introduction

The aim of these pages is to give a brief, self-contained introduction to that part of geometric measure theory which is more directly related to the calculus of variations, namely the theory of currents and its applications to the solution of Plateau problem. (The theory of finite-perimeter sets, which is closely related to currents and to the Plateau problem, is treated in the article Free Interfaces and Free Discontinuities: Variational Problems in the Encyclopedia.)

Named after the Belgian physicist JAF Plateau (1801–1883), this problem was originally formulated as follows: find the surface of minimal area spanning a given curve in the space. Nowadays, it is mostly intended in the sense of developing a mathematical framework where the existence of k -dimensional surfaces of minimal volume that span a prescribed boundary can be rigorously proved. Indeed, several solutions have been proposed in the last century, none of which is completely satisfactory.

One difficulty is that the infimum of the area among all smooth surfaces with a certain boundary may not be attained. More precisely, it may happen that all minimizing sequences (i.e., sequences of smooth surfaces whose area approaches the infimum) converge to a singular surface. Therefore, one is forced to consider a larger class of admissible surfaces than just smooth ones (in fact, one might want to do this also for modeling reasons – this is indeed the case with soap films, soap bubbles, and other capillarity problems). But what does it mean that a set “spans” a

given curve? and what should we intend by area of a set which is not a smooth surface?

The theory of integral currents developed by Federer and Fleming (1960) provides a class of generalized (oriented) surfaces with well-defined notions of boundary and area (called mass) where the existence of minimizers can be proved by direct methods. More precisely, this class is large enough to have good compactness properties with respect to a topology that makes the mass a lower-semicontinuous functional. This approach turned out to be quite powerful and flexible, and in the last decades the theory of currents has found applications in several different areas, from dynamical systems (in particular, Mather theory) to the theory of foliations, to optimal transport problems.

Hausdorff Measures, Dimension, and Rectifiability

The volume of a smooth d -dimensional surface in \mathbb{R}^n is usually defined using parametrizations by subsets of \mathbb{R}^d . The notion of Hausdorff measure allows to compute the d -dimensional volume using coverings instead of parametrizations, and, what is more important, applies to all sets in \mathbb{R}^n , and makes sense even if d is not an integer. Attached to Hausdorff measure is the notion of Hausdorff dimension. Again, it can be defined for all sets in \mathbb{R}^n and is not necessarily an integer. The last fundamental notion is rectifiability: k -rectifiable sets can be roughly understood as the largest class of k -dimensional sets for which it is still possible to define a k -dimensional tangent bundle, even if only in a very weak sense. They are essential to the construction of integral currents.

Hausdorff Measure

Let $d \geq 0$ be a positive real number. Given a set E in \mathbb{R}^n , for every $\delta > 0$ we set

$$\mathcal{H}_\delta^d(E) := \frac{\omega_d}{2^d} \inf \left\{ \sum_i (\text{diam}(E_i))^d \right\} \quad [1]$$

where ω_d is the d -dimensional volume of the unit ball in \mathbb{R}^d whenever d is an integer (there is no canonical choice for ω_d when d is not an integer; a convenient one is $\omega_d = 2^d$), and the infimum is taken over all countable families of sets $\{E_i\}$ that cover E and whose diameters satisfy $\text{diam}(E_i) \leq \delta$. The d -dimensional Hausdorff measure of E is

$$\mathcal{H}^d(E) := \lim_{\delta \rightarrow 0} \mathcal{H}_\delta^d(E) \quad [2]$$

(the limit exists because $\mathcal{H}_\delta^d(E)$ is decreasing in δ).

Remarks

(i) \mathcal{H}^d is called d -dimensional because of its scaling behavior: if E_λ is a copy of E scaled homothetically by a factor λ , then

$$\mathcal{H}^d(E_\lambda) = \lambda^d \mathcal{H}^d(E)$$

Thus, \mathcal{H}^1 scales like the length, \mathcal{H}^2 scales like the area, and so on.

(ii) The measure \mathcal{H}^d is clearly invariant under rigid motions (translations and rotations). This implies that \mathcal{H}^d agrees on \mathbb{R}^d with the Lebesgue measure up to some constant factor; the renormalization constant $\omega_d/2^d$ in [1] makes this factor equal to 1. Thus, $\mathcal{H}^d(E)$ agrees with the usual d -dimensional volume for every set E in \mathbb{R}^d , and the area formula shows that the same is true if E is (a subset of) a d -dimensional surface of class C^1 in \mathbb{R}^n .

(iii) Besides the Hausdorff measure, there are several other, less popular notions of d -dimensional measure: all of them are invariant under rigid motion, scale in the expected way, and agree with \mathcal{H}^d for sets contained in \mathbb{R}^d or in a d -dimensional surface of class C^1 , and yet they differ for other sets (for further details, see Federer (1996, section 2.10)).

(iv) The definition of $\mathcal{H}^d(E)$ uses only the notion of diameter, and therefore makes sense when E is a subset of an arbitrary metric space. Note that $\mathcal{H}^d(E)$ depends only on the restriction of the metric to E , and not on the ambient space.

(v) The measure \mathcal{H}^d is countably additive on the σ -algebra of Borel sets in \mathbb{R}^n , but not on all sets; to avoid pathological situations, we shall always assume that sets and maps are Borel measurable.

Hausdorff Dimension

According to intuition, the length of a surface should be infinite, while the area of a curve should be null. These are indeed particular cases of the following implications:

$$\mathcal{H}^d(E) > 0 \Rightarrow \mathcal{H}^{d'}(E) = \infty \quad \text{for } d' < d$$

$$\mathcal{H}^d(E) < \infty \Rightarrow \mathcal{H}^{d'}(E) = 0 \quad \text{for } d' > d$$

Hence, the infimum of all d such that $\mathcal{H}^d(E) = 0$ and the supremum of all d such that $\mathcal{H}^d(E) = \infty$ coincide. This number is called Hausdorff dimension of E , and denoted by $\dim_H(E)$. For surface of class C^1 , the notion of Hausdorff dimension agrees with the usual one. Example of sets with nonintegral dimension are described in the next subsection.

Remarks

(i) Note that $\mathcal{H}^d(E)$ may be 0 or ∞ even for $d = \dim_H(E)$.

(ii) The Hausdorff dimension of a set E is strictly related to the metric on E , and not just to the topology. Indeed, it is preserved under diffeomorphisms but not under homeomorphisms, and it does not always agree with the topological dimension. For instance, the Hausdorff dimension of the graph of a continuous function $f: \mathbb{R} \rightarrow \mathbb{R}$ can be any number between 1 and 2 (included).

(iii) For nonsmooth sets, the Hausdorff dimension does not always conform to intuition: for example, the dimension of a Cartesian product $E \times F$ of compact sets does not agree in general with the sum of the dimensions of E and F .

(iv) There are many other notions of dimension besides Hausdorff and topological ones. Among these, packing dimension and box-counting dimension have interesting applications (see Falconer (2003, chapters 3 and 4)).

Self-Similar Fractals

Interesting examples of sets with nonintegral dimension are self-similar fractals. We present here a simplified version of a construction due to Hutchinson (Falconer 2003, chapter 9). Let $\{\Psi_i\}$ be a finite set of similitudes of \mathbb{R}^n with scaling factor $\lambda_i < 1$, and assume that there exists a bounded open set V such that the sets $V_i := \Psi_i(V)$ are pairwise disjoint and contained in V . The self-similar fractal associated with the system $\{\Psi_i\}$ is the compact set C that satisfies

$$C = \bigcup_i \Psi_i(C) \quad [3]$$

The term “self-similar” follows by the fact that C can be written as a union of scaled copies of itself.

The existence (and uniqueness) of such a C follows from a standard fixed-point argument applied to the map $C \mapsto \bigcup \Psi_i(C)$. The dimension d of C is the unique solution of the equation

$$\sum_i \lambda_i^d = 1 \quad [4]$$

Formula [4] can be easily justified: if the sets $\Psi_i(C)$ are disjoint – and the assumption on V implies that this is almost the case – then [3] implies $\mathcal{H}^d(C) = \sum \mathcal{H}^d(\Psi_i(C)) = \sum \lambda_i^d \mathcal{H}^d(C)$, and therefore $\mathcal{H}^d(C)$ can be positive and finite if and only if d satisfies [4].

An example of this construction is the usual Cantor set in \mathbb{R} , which is given by the similitudes

$$\Psi_1(x) := \frac{1}{3}x \text{ and } \Psi_2(x) := \frac{2}{3} + \frac{1}{3}x$$

By [4], its dimension is $d = \log 2 / \log 3$. Other examples are described in Figures 1–3.

Rectifiable Sets

Given an integer $k = 1, \dots, n$, we say that a set E in \mathbb{R}^n is k -rectifiable if it can be covered by a countable family of sets $\{S_j\}$ such that S_0 is \mathcal{H}^k -negligible (i.e., $\mathcal{H}^k(S_0) = 0$) and S_j is a k -dimensional surface of class C^1 for $j = 1, 2, \dots$. Note that $\dim_{\mathcal{H}}(E) \leq k$ because each S_j has dimension k .

A k -rectifiable set E bears little resemblance to smooth surfaces (it can be everywhere dense!), but it still admits a suitably weak notion of tangent bundle.

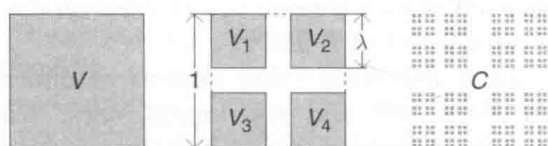


Figure 1 The maps $\Psi_i, i = 1, \dots, 4$, take the square V into the squares V_i at the corners of V . The scaling factor is λ for all i , hence $\dim_{\mathcal{H}}(C) = \log 4 / (-\log \lambda)$. Note that $\dim_{\mathcal{H}}(C)$ can be any number between 0 and 2, including 1.

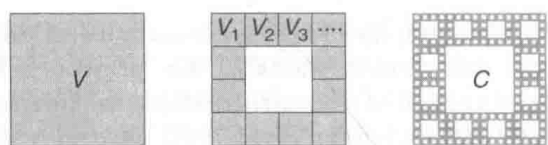


Figure 2 A self-similar fractal with more complicated topology. The scaling factor is $1/4$ for all twelve similitudes, hence $\dim_{\mathcal{H}}(C) = \log 12 / \log 4$.

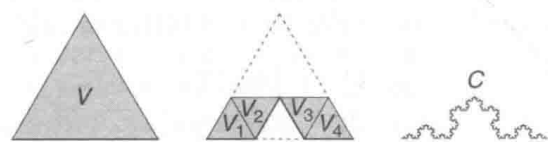


Figure 3 The von Koch curve (or snowflake). The scaling factor is $1/3$ for all four similitudes, hence $\dim_{\mathcal{H}}(C) = \log 4 / \log 3$.

More precisely, it is possible to associate with every $x \in E$ a k -dimensional subspace of \mathbb{R}^n , denoted by $\text{Tan}(E, x)$, so that for every k -dimensional surface S of class C^1 in \mathbb{R}^n there holds

$$\text{Tan}(E, x) = \text{Tan}(S, x) \text{ for } \mathcal{H}^k\text{-a.e. } x \in E \cap S \quad [5]$$

where $\text{Tan}(S, x)$ is the tangent space to S at x according to the usual definition.

It is not difficult to see that $\text{Tan}(E, x)$ is uniquely determined by [5] up to an \mathcal{H}^k -negligible amount of points $x \in E$, and if E is a surface of class C^1 , then it agrees with the usual tangent space for \mathcal{H}^k -almost all points of E .

Remarks

(i) In the original definition of rectifiability, the sets S_j with $j > 0$ are Lipschitz images of \mathbb{R}^k , that is, $S_j := f_j(\mathbb{R}^k)$, where $f_j: \mathbb{R}^k \rightarrow \mathbb{R}^n$ is a Lipschitz map. It can be shown that this definition is equivalent to the one above.

(ii) The construction of the tangent bundle is straightforward: Let $\{S_j\}$ be a covering of E as earlier, and set $\text{Tan}(E, x) := \text{Tan}(S_j, x)$, where j is the smallest positive integer such that $x \in S_j$. Then [5] is an immediate corollary of the following lemma: if S and S' are k -dimensional surfaces of class C^1 in \mathbb{R}^n , then $\text{Tan}(S, x) = \text{Tan}(S', x)$ for \mathcal{H}^k -almost every $x \in S \cap S'$.

(iii) A set E in \mathbb{R}^n is called purely k -unrectifiable if it contains no k -rectifiable subset with positive k -dimensional measure, or, equivalently, if $\mathcal{H}^k(E \cap S) = 0$ for every k -dimensional surface S of class C^1 . For instance, every product $E := E_1 \times E_2$, where E_1 and E_2 are \mathcal{H}^1 -negligible sets in \mathbb{R} is a purely 1-unrectifiable set in \mathbb{R}^2 (it suffices to show that $\mathcal{H}^1(E \cap S) = 0$ whenever S is the graph of a function $f: \mathbb{R} \rightarrow \mathbb{R}$ of class C^1 , and this follows by the usual formula for the length of the graph). Note that the Hausdorff dimension of such product sets can be any number between 0 and 2, hence rectifiability is not related to dimension. The self-similar fractals described in Figures 1 and 3 are both purely 1-unrectifiable.

Rectifiable Sets with Finite Measure

If E is a k -rectifiable set with finite (or locally finite) k -dimensional measure, then $\text{Tan}(E, x)$ can be related to the behavior of E close to the point x .

Let $B(x, r)$ be the open ball in \mathbb{R}^n with center x and radius r , and let $C(x, T, a)$ be the cone with center x , axis T – a k -dimensional subspace of \mathbb{R}^n – and amplitude $\alpha = \arcsin a$, that is,

$$C(x, T, a) := \{x' \in \mathbb{R}^n: \text{dist}(x' - x, T) \leq a|x' - x|\}$$

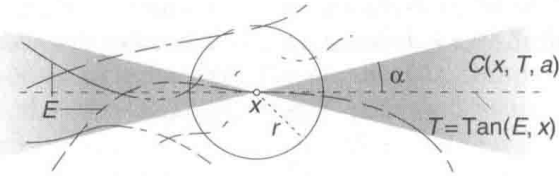


Figure 4 A rectifiable set E close to a point x of approximate tangency. The part of E contained in the ball $B(x, r)$ but not in the cone $C(x, T, a)$ is not empty, but only small in measure.

For \mathcal{H}^k -almost every $x \in E$, the measure of $E \cap B(x, r)$ is asymptotically equivalent, as $r \rightarrow 0$, to the measure of a flat disk of radius r , that is,

$$\mathcal{H}^k(E \cap B(x, r)) \sim \omega_k r^k$$

Moreover, the part of E contained in $B(x, r)$ is mostly located close to the tangent plane $\text{Tan}(E, x)$, that is,

$$\mathcal{H}^k(E \cap B(x, r) \cap C(x, \text{Tan}(E, x), a)) \sim \omega_k r^k$$

for every $a > 0$

When this condition holds, $\text{Tan}(E, x)$ is called the approximate tangent space to E at x (see Figure 4).

The Area Formula

The area formula allows to compute the measure $\mathcal{H}^k(\Phi(E))$ of the image of a set E in \mathbb{R}^k as the integral over E of a suitably defined Jacobian determinant of Φ . When Φ is injective and takes values in \mathbb{R}^k , we recover the usual change of variable formula for multiple integrals.

We consider first the linear case. If L is a linear map from \mathbb{R}^k to \mathbb{R}^m with $m \geq k$, the volume ratio $\rho := \mathcal{H}^k(L(E))/\mathcal{H}^k(E)$ does not depend on E , and agrees with $|\det(PL)|$, where P is any linear isometry from the image of L into \mathbb{R}^k , and $\det(PL)$ is the determinant of the $k \times k$ matrix associated with PL . The volume ratio ρ can be computed using one of the following identities:

$$\rho = \sqrt{\det(L^*L)} = \sqrt{\sum (\det M)^2} \quad [6]$$

where L^* is the adjoint of L (thus, L^*L is a linear map from \mathbb{R}^k into \mathbb{R}^k), and the sum in the last term is taken over all $k \times k$ minors M of the matrix associated with L .

Let $\Phi: \mathbb{R}^k \rightarrow \mathbb{R}^m$ be a map of class C^1 with $m \geq k$, and E a set in \mathbb{R}^k . Then

$$\int_{\Phi(E)} \#(\Phi^{-1}(y) \cap E) d\mathcal{H}^k(y) = \int_E J(x) d\mathcal{H}^k(x) \quad [7]$$

where $\#A$ stands for the number of elements of A , and the Jacobian J is

$$J(x) := \sqrt{\det(\nabla\Phi(x)^* \nabla\Phi(x))} \quad [8]$$

Note that the left-hand side of [7] is $\mathcal{H}^k(\Phi(E))$ when Φ is injective.

Remark

Formula [7] holds even if E is a k -rectifiable set in \mathbb{R}^n . In this case, the gradient $\nabla\Phi(x)$ in [8] should be replaced by the tangential derivative of Φ at x (viewed as a linear map from $\text{Tan}(E, x)$ into \mathbb{R}^m). No version of formula [7] is available when E is not rectifiable.

Vectors, Covectors, and Differential Forms

In this section, we review some basic notions of multilinear algebra. We have chosen a definition of k -vectors and k -covectors in \mathbb{R}^n , and of the corresponding exterior products, which is quite convenient for computations, even though not as satisfactory from the formal viewpoint. The main drawback is that it depends on the choice of a standard basis of \mathbb{R}^n , and therefore cannot be used to define forms (and currents) when the ambient space is a general manifold.

k -Vectors and Exterior Product

Let $\{e_1, \dots, e_n\}$ be the standard basis of \mathbb{R}^n . Given an integer $k \leq n$, $I(n, k)$ is the set of all multi-indices $i = (i_1, \dots, i_k)$ with $1 \leq i_1 < i_2 < \dots < i_k \leq n$, and for every $i \in I(n, k)$ we introduce the expression

$$e_i = e_{i_1} \wedge e_{i_2} \wedge \dots \wedge e_{i_k}$$

A k -vector in \mathbb{R}^n is any formal linear combination $\sum \alpha_i e_i$ with $\alpha_i \in \mathbb{R}$ for every $i \in I(n, k)$. The space of k -vectors is denoted by $\wedge_k(\mathbb{R}^n)$; in particular, $\wedge_1(\mathbb{R}^n) = \mathbb{R}^n$. For reasons of formal convenience, we set $\wedge_0(\mathbb{R}^n) := \mathbb{R}$ and $\wedge_k(\mathbb{R}^n) := \{0\}$ for $k > n$.

We denote by $|\cdot|$ the Euclidean norm on $\wedge_k(\mathbb{R}^n)$.

The exterior product $v \wedge w \in \wedge_{k+b}(\mathbb{R}^n)$ is defined for every $v \in \wedge_k(\mathbb{R}^n)$ and $w \in \wedge_b(\mathbb{R}^n)$, and is completely determined by the following properties: (1) associativity, (2) linearity in both arguments, and (3) $e_i \wedge e_j = -e_j \wedge e_i$ for every $i \neq j$ and $e_i \wedge e_i = 0$ for every i .

Simple Vectors and Orientation

A simple k -vector is any v in $\wedge_k(\mathbb{R}^n)$ that can be written as a product of 1-vectors, that is,

$$v = v_1 \wedge v_2 \wedge \dots \wedge v_k$$

It can be shown that v is null if and only if the vectors $\{v_i\}$ are linearly dependent. If v is not null,

then it is uniquely determined by the following objects: (1) the k -dimensional space M spanned by $\{v_i\}$; (2) the orientation of M associated with the basis $\{v_i\}$; (3) the euclidean norm $|v|$. In particular, M does not depend on the choice of the vectors v_i . Note that $|v|$ is equal to the k -dimensional volume of the parallelogram spanned by $\{v_i\}$.

Hence, the map $v \mapsto M$ is a one-to-one correspondence between the class of simple k -vectors with norm $|v|=1$ and the Grassmann manifold of oriented k -dimensional subspaces of \mathbb{R}^n .

This remark paves the way to the following definition: if S is a k -dimensional surface of class C^1 in \mathbb{R}^n , possibly with boundary, an orientation of S is a continuous map $\tau_S: S \rightarrow \wedge_k(\mathbb{R}^n)$ such that $\tau_S(x)$ is a simple k -vector with norm 1 that spans $\text{Tan}(S, x)$ for every x . With every orientation of S (if any exists) is canonically associated the orientation of the boundary ∂S that satisfies

$$\tau_S(x) = \eta(x) \wedge \tau_{\partial S}(x) \quad \text{for every } x \in \partial S \quad [9]$$

where $\eta(x)$ is the inner normal to ∂S at x .

k -Covectors

The standard basis of the dual of \mathbb{R}^n is $\{dx_1, \dots, dx_n\}$, where $dx_i: \mathbb{R}^n \rightarrow \mathbb{R}$ is the linear functional that takes every $x = (x_1, \dots, x_n)$ into the i th component x_i . For every $i \in I(n, k)$ we set

$$dx_i = dx_{i_1} \wedge dx_{i_2} \wedge \dots \wedge dx_{i_k}$$

and the space $\wedge^k(\mathbb{R}^n)$ of k -covectors consists of all formal linear combinations $\sum \alpha_i dx_i$. The exterior product of covectors is defined as that for vectors. The space $\wedge^k(\mathbb{R}^n)$ is dual to $\wedge_k(\mathbb{R}^n)$ via the duality pairing $\langle ; \rangle$ defined by the relations $\langle dx_i; e_j \rangle := \delta_{ij}$ (that is, 1 if $i=j$ and 0 otherwise).

Differential Forms and Stokes Theorem

A differential form of order k on \mathbb{R}^n is a map $\omega: \mathbb{R}^n \rightarrow \wedge^k(\mathbb{R}^n)$. Using the canonical basis of $\wedge^k(\mathbb{R}^n)$, we can write ω as

$$\omega(x) = \sum_{i \in I(n, k)} \omega_i(x) dx_i$$

where the coordinates ω_i are real functions on \mathbb{R}^n . The exterior derivative of a k -form ω of class C^1 is the $(k+1)$ -form

$$d\omega(x) := \sum_{i \in I(n, k)} d\omega_i(x) \wedge dx_i$$

where, for every scalar function f , df is the 1-form

$$df(x) := \sum_{i=1}^n \frac{\partial f}{\partial x_i}(x) dx_i$$

If S is a k -dimensional oriented surface, the integral of a k -form ω on S is naturally defined by

$$\int_S \omega := \int_S \langle \omega(x); \tau_S(x) \rangle d\mathcal{H}^k(x)$$

Stokes theorem states that for every $(k-1)$ -form ω of class C^1 there holds

$$\int_{\partial S} \omega = \int_S d\omega \quad [10]$$

provided that ∂S is endowed with the orientation $\tau_{\partial S}$ that satisfies [9].

Currents

The definition of k -dimensional currents closely resembles that of distributions: they are the dual of smooth k -forms with compact support. Since every oriented k -dimensional surface defines by integration a linear functional on forms, currents can be regarded as generalized oriented surfaces. As every distribution admits a derivative, so every current admits a boundary. Indeed, many other basic notions of homology theory can be naturally extended to currents – this was actually one of the motivations behind the introduction of currents, due to de Rham.

For the applications to variational problems, smaller classes of currents are usually considered; the most relevant to the Plateau problem is that of integral currents. Note that the definitions of the spaces of normal, rectifiable, and integral currents and the symbols used to denote them vary, sometimes more than slightly, depending on the author.

Currents, Boundary, and Mass

Let n, k be integers with $n \geq k$. The space of k -dimensional currents on \mathbb{R}^n , denoted by $\mathcal{D}_k(\mathbb{R}^n)$, is the dual of the space $\mathcal{D}^k(\mathbb{R}^n)$ of smooth k -forms with compact support in \mathbb{R}^n . For $k \geq 1$, the boundary of a k -current T is the $(k-1)$ -current ∂T defined by

$$\langle \partial T; \omega \rangle := \langle T; d\omega \rangle \quad \text{for every } \omega \in \mathcal{D}^{k-1}(\mathbb{R}^n) \quad [11]$$

while the boundary of a 0-current is set equal to 0. The mass of T is the number

$$\mathbb{M}(T) := \sup \left\{ \langle T; \omega \rangle : \omega \in \mathcal{D}^k(\mathbb{R}^n), |\omega| \leq 1 \right\} \quad [12]$$

Fundamental examples of k -currents are oriented k -dimensional surfaces: with each oriented surface S of class C^1 is canonically associated the current $\langle T; d\omega \rangle := \int_S \omega$ (in fact, S is completely determined by the action on forms, i.e., by the associated

current). By Stokes theorem, the boundary of T is the current associated with the boundary of S ; thus, the notion of boundary for currents is compatible with the classical one for oriented surfaces. A simple computation shows that $M(T) = \mathcal{H}^k(S)$; therefore, the mass provides a natural extension of the notion of k -dimensional volume to k -currents.

Remarks

(i) Not all k -currents look like k -dimensional surfaces. For example, every k -vectorfield $v: \mathbb{R}^n \rightarrow \wedge_k(\mathbb{R}^n)$ defines by duality the k -current

$$\langle T; \omega \rangle := \int \langle \omega(x); v(x) \rangle d\mathcal{H}^n(x)$$

The mass of T is $\int |v| d\mathcal{H}^n$, and the boundary is represented by a similar integral formula involving the partial derivatives of v (in particular, for 1-vectorfields, the boundary is the 0-current associated with the divergence of v). Note that the dimension of such T is k because k -vectorfields act on k -forms, and there is no relation with the dimension of the support of T , which is n .

(ii) To be precise, $\mathcal{D}^k(\mathbb{R}^n)$ is a locally convex topological vector space, and $\mathcal{D}_k(\mathbb{R}^n)$ is its topological dual. As such, $\mathcal{D}_k(\mathbb{R}^n)$ is endowed with a dual (or weak*) topology. We say that a sequence of k -currents (T_j) converge to T if they converge in the dual topology, that is,

$$\langle T_j; \omega \rangle \rightarrow \langle T; \omega \rangle \quad \text{for every } \omega \in \mathcal{D}^k(\mathbb{R}^n) \quad [13]$$

Recalling the definition of mass, it is easy to show that it is lower-semicontinuous with respect the dual topology, and in particular

$$\liminf M(T_j) \geq M(T) \quad [14]$$

Currents with Finite Mass

By definition, a k -current T with finite mass is a linear functional on k -forms which is bounded with respect to the supremum norm, and by Riesz theorem it can be represented as a bounded measure with values in $\wedge_k(\mathbb{R}^n)$. In other words, there exist a finite positive measure μ on \mathbb{R}^n and a density function $\tau: \mathbb{R}^n \rightarrow \wedge_k(\mathbb{R}^n)$ such that $|\tau(x)| = 1$ for every x and

$$\langle T; \omega \rangle = \int \langle \omega(x); \tau(x) \rangle d\mu(x)$$

The fact that currents are the dual of a separable space yields the following compactness result: a

sequence of k -currents (T_j) with uniformly bounded masses $M(T_j)$ admits a subsequence that converges to a current with finite mass.

Normal Currents

A k -current T is called normal if both T and ∂T have finite mass. The compactness result stated in the previous paragraph implies the following compactness theorem for normal currents: a sequence of normal currents (T_j) with $M(T_j)$ and $M(\partial T_j)$ uniformly bounded admits a subsequence that converges to a normal current.

Rectifiable Currents

A k -current T is called rectifiable if it can be represented as

$$\langle T; \omega \rangle = \int_E \langle \omega(x); \tau(x) \rangle \theta(x) d\mathcal{H}^k(x)$$

where E is a k -rectifiable set, τ is an orientation of E – that is, $\tau(x)$ is a simple unit k -vector that spans $\text{Tan}(E, x)$ for \mathcal{H}^k -almost every $x \in E$ – and θ is a real function such that $\int_E |\theta| d\mathcal{H}^k$ is finite, called multiplicity. Such T is denoted by $T = [E, \tau, \theta]$. In particular, a rectifiable 0-current can be written as $\langle T; \omega \rangle = \sum \theta_i \omega(x_i)$, where $E = \{x_i\}$ is a countable set in \mathbb{R}^n and $\{\theta_i\}$ is a sequence of real numbers with $\sum |\theta_i| < +\infty$.

Integral Currents

If T is a rectifiable current and the multiplicity θ takes integral values, T is called an integer multiplicity rectifiable current. If both T and ∂T are integer multiplicity rectifiable currents, then T is an integral current.

The first nontrivial result is the boundary rectifiability theorem: if T is an integer multiplicity rectifiable current and ∂T has finite mass, then ∂T is an integer multiplicity rectifiable current, too, and therefore T is an integral current.

The second fundamental result is the compactness theorem for integral currents: a sequence of integral currents (T_j) with $M(T_j)$ and $M(\partial T_j)$ uniformly bounded admits a subsequence that converges to an integral current.

Remarks

(i) The point of the compactness theorem for integral currents is not the existence of a converging subsequence – that being already established by the compactness theorem for normal currents – but the fact that the limit is an integral current. In fact, this result is often referred to as a “closure theorem” rather than a “compactness theorem.”

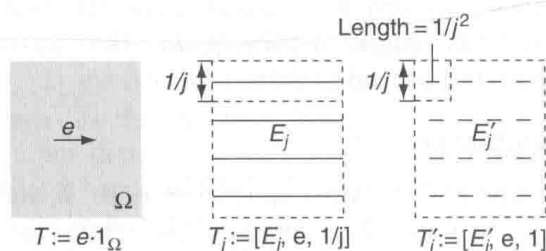


Figure 5 T is the normal 1-current on \mathbb{R}^2 associated with the vectorfield equal to the unit vector e on the unit square Ω , and equal to 0 outside. T_j are the rectifiable currents associated with the sets E_j (middle) and the constant multiplicity $1/j$, and then $\mathbb{M}(T_j)=1, \mathbb{M}(\partial T_j)=2$. T'_j are the integral currents associated with the sets E'_j (left) and the constant multiplicity 1, and then $\mathbb{M}(T'_j)=1, \mathbb{M}(\partial T'_j)=2j^2$. Both (T_j) and (T'_j) converge to T .

(ii) The following observations may clarify the role of assumptions in the compactness theorem: (1) a sequence of integral currents (T_j) with $\mathbb{M}(T_j)$ uniformly bounded – but not $\mathbb{M}(\partial T_j)$ – may converge to any current with finite mass, not necessarily a rectifiable one. (2) A sequence of rectifiable currents (T_j) with rectifiable boundaries and $\mathbb{M}(T_j), \mathbb{M}(\partial T_j)$ uniformly bounded may converge to any normal current, not necessarily a rectifiable one. Examples of both situations are described in Figure 5.

Application to the Plateau Problem

The compactness result for integral currents implies the existence of currents with minimal mass: if Γ is the boundary of an integral k -current in $\mathbb{R}^n, 1 \leq k \leq n$, then there exists a current T of minimal mass among those that satisfy $\partial T = \Gamma$.

The proof of this existence result is a typical example of the direct method: let m be the infimum of $\mathbb{M}(T)$ among all integral currents with boundary Γ , and let (T_j) be a minimizing sequence (i.e., a sequence of integral currents with boundary Γ such that $\mathbb{M}(T_j)$ converges to m). Since $\mathbb{M}(T_j)$ is bounded and $\mathbb{M}(\partial T_j) = \mathbb{M}(\Gamma)$ is constant, we can apply the compactness theorem for integral currents and extract a subsequence of (T_j) that converges to an integral current T . By the continuity of the boundary operator, $\partial T = \lim \partial T_j = \Gamma$, and by the semicontinuity of the mass $\mathbb{M}(T) \leq \lim \mathbb{M}(T_j) = m$ (cf. [14]). Thus, T is the desired minimal current.

Remarks

(i) Every integral $(k-1)$ -current Γ with null boundary and compact support in \mathbb{R}^n is the boundary of an integral current, and therefore is an admissible datum for the previous existence result.

(ii) A mass-minimizing integral current T is more regular than a general integral current. For $k = n-1$, there exists a closed singular set S with $\dim_{\mathbb{H}}(S) \leq$

$k-7$ such that T agrees with a smooth surface in the complement of S and of the support of the boundary. In particular, T is smooth away from the boundary for $n \leq 7$. For general k , it can only be proved that $\dim_{\mathbb{H}}(S) \leq k-2$. Both results are optimal: in $\mathbb{R}^4 \times \mathbb{R}^4$, the minimal 7-current with boundary $\Gamma := \{|x|=|y|=1\}$ – a product of two 3-spheres – is the cone $T := \{|x|=|y| \leq 1\}$, and is singular at the origin. In $\mathbb{R}^2 \times \mathbb{R}^2$, the minimal 2-current with boundary $\Gamma := \{x=0, |y|=1\} \cup \{y=0, |x|=1\}$ – a union of two disjoint circles – is the union of the disks $\{x=0, |y| \leq 1\} \cup \{y=0, |x| \leq 1\}$, and is singular at the origin.

(iii) In certain cases, the mass-minimizing current T may not agree with the solution of the Plateau problem suggested by intuition. The first reason is that currents do not include nonorientable surfaces, which sometimes may be more convenient (Figure 6). Another reason is that the mass of an integral current T associated with a k -rectifiable set E does not agree with the measure $\mathcal{H}^k(E)$ – called size of T – because multiplicity must be taken into account, and for certain Γ the mass-minimizing current may be not size-minimizing (Figure 7). Unfortunately, proving the existence of size-minimizing currents is much more complicated, due to lack of suitable compactness theorems.

(iv) For $k=2$, the classical approach to the Plateau problem consists in parametrizing surfaces in \mathbb{R}^n by maps f from a given two-dimensional domain D into \mathbb{R}^n , and looking for minimizers of the area functional

$$\int_D \sqrt{\det(\nabla f^* \nabla f)}$$



Figure 6 The surface with minimal area spanning the (oriented) curve Γ is the Möbius strip Σ . However, Σ is not orientable, and cannot be viewed as a current. The mass-minimizing current with boundary Γ is Σ' .

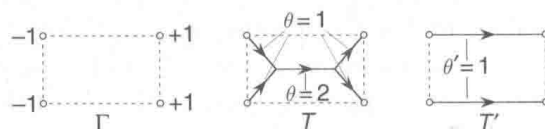


Figure 7 The boundary Γ is a 0-current associated with four oriented points. The size (length) of T is smaller than that of T' . However, $\partial T = \Gamma$ implies that the multiplicity of T must be 2 on the central segment and 1 on the others; thus the mass of T is larger than its size. The size-minimizing current with boundary Γ is T , while the mass-minimizing one is T' .

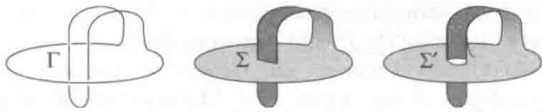


Figure 8 The surface Σ minimizes the area among surfaces parametrized by the disk with boundary Γ . The mass-minimizing current Σ' can only be parametrized by a disk with a handle. Note that Σ is a singular surface, while Σ' is not.

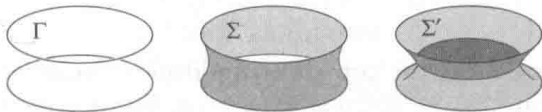


Figure 9 Two possible soap films spanning the wire Γ : unlike Σ , Σ' cannot be viewed as a current with multiplicity 1 and boundary Γ .

(recall the area formula, discussed earlier) under the constraint $f(\partial D) = \Gamma$. In this framework, the choice of the domain D prescribes the topological type of admissible surfaces, and therefore the minimizer may differ substantially from the mass-minimizing current with boundary Γ (Figure 8).

(v) For some modeling problems, for instance, those related to soap films and soap bubbles, currents do not provide the right framework (Figure 9). A possible alternative are integral varifolds (cf. Almgren 2001). However, it should be pointed out that this framework does not allow for “easy” application of the direct method, and the existence of minimal varifolds is in general quite difficult to prove.

Miscellaneous Results and Useful Tools

(i) An important issue, related to the use of currents for solving variational problems, concerns the extent to which integral currents can be approximated by regular objects. For many reasons, the “right” regular class to consider are not smooth surfaces, but integral polyhedral currents, that is, linear combinations with integral coefficients of oriented simplexes. The following approximation theorem holds: for every integral current T in \mathbb{R}^n there exists a sequence of integral polyhedral currents (T_j) such that

$$\begin{aligned} T_j &\rightarrow T, \quad \partial T_j \rightarrow \partial T \\ \mathbf{M}(T_j) &\rightarrow \mathbf{M}(T), \quad \mathbf{M}(\partial T_j) \rightarrow \mathbf{M}(\partial T) \end{aligned}$$

The proof is based on a quite useful tool, called polyhedral deformation.

(ii) Many geometric operations for surfaces have an equivalent for currents. For instance, it is possible to define the image of a current in \mathbb{R}^n via a smooth proper map $f: \mathbb{R}^n \rightarrow \mathbb{R}^m$. Indeed, with every k -form ω on \mathbb{R}^m is canonically associated a k -form $f^\# \omega$ on \mathbb{R}^n , called pullback of ω according to f . The adjoint of the

pullback is an operator, called push-forward, that takes every k -current T in \mathbb{R}^n into a k -current $f_\# T$ in \mathbb{R}^m . If T is the rectifiable current associated with a rectifiable set E and a multiplicity θ , the push-forward $f_\# T$ is the rectifiable current associated with $f(E)$ – and a multiplicity $\theta'(y)$ which is computed by adding up with the right sign all $\theta(x)$ with $x \in f^{-1}(y)$. As one might expect, the boundary of the push-forward is the push-forward of the boundary.

(iii) In general, it is not possible to give a meaning to the intersection of two currents, and not even of a current and a smooth surface. However, it is possible to define the intersection of a normal k -current T and a level surface $f^{-1}(y)$ of a smooth map $f: \mathbb{R}^n \rightarrow \mathbb{R}^b$ (with $k \leq b \leq n$) for almost every y , resulting in a current T_y with the expected dimension $b - k$. This operation is called slicing.

(iv) When working with currents, a quite useful notion is that of flat norm:

$$\mathbf{F}(T) := \inf \{ \mathbf{M}(R) + \mathbf{M}(S) : T = R + \partial S \}$$

where T and R are k -currents, and S is a $(k+1)$ -current. The relevance of this notion lies in the fact that a sequence (T_j) that converges with respect to the flat norm converges also in the dual topology, and the converse holds if the masses $\mathbf{M}(T_j)$ and $\mathbf{M}(\partial T_j)$ are uniformly bounded. Hence, the flat norm metrizes the dual topology of currents (at least on sets of currents where the mass and the mass of the boundary are bounded).

Since $\mathbf{F}(T)$ can be explicitly estimated from above, it can be quite useful in proving that a sequence of currents converges to a certain limit. Finally, the flat norm gives a (geometrically significant) measure of how far apart two currents are: for instance, given the 0-currents δ_x and δ_y (the Dirac masses at x and y , respectively), then $\mathbf{F}(\delta_x - \delta_y)$ is exactly the distance between x and y .

See also: Free Interfaces and Free Discontinuities; Variational Problems; Γ -Convergence and Homogenization; Geometric Phases; Image Processing; Mathematics; Minimal Submanifolds; Mirror Symmetry; A Geometric Survey; Moduli Spaces: An Introduction.

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Geometric Phases

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Introduction

We invite the reader to perform the following simple experiment. Put your arm out in front of you keeping your thumb pointing up perpendicular to your arm. Move your arm up over your head, then bring it down to your side, and at last bring the arm back in front of you again. In this experiment an object (your thumb) was taken along a closed path traced by another object (your arm) in a way that a simple local law of transport was applied. In this case the local law consisted of two ingredients: (1) preserve the orthogonality of your thumb with respect to your arm and (2) do not rotate the thumb about its instantaneous axis (i.e., your arm). Performing the experiment in this way, you will manage to avoid rotations of your thumb locally; however, in the end you will experience a rotation of 90° globally.

The experiment above can be regarded as the archetypical example of the phenomenon called anholonomy by physicists and holonomy by mathematicians. In this article, we consider the manifestation of this phenomenon in the realm of quantum theory. The objects to be transported along closed paths in suitable manifolds will be wave functions representing quantum systems. After applying local laws dictated by inputs coming from physics, one ends up with a new wave function that has picked up a complex phase factor. Phases of this kind are called geometric phases, with the famous Berry phase being a special case.

The Space of Rays

Let us consider a quantum system with physical states represented by elements $|\psi\rangle$ of some Hilbert space \mathcal{H} with scalar product $\langle \cdot | \cdot \rangle : \mathcal{H} \times \mathcal{H} \rightarrow \mathbb{C}$. For simplicity, we assume that \mathcal{H} is finite dimensional, $\mathcal{H} \simeq \mathbb{C}^{n+1}$ with $n \geq 1$. The infinite-dimensional case can be studied by taking the inductive limit $n \rightarrow \infty$.

Let us denote the complex amplitudes characterizing the state $|\psi\rangle$ by Z^α , $\alpha = 0, 1, \dots, n$. For a normalized state,

$$\|\psi\|^2 = \langle \psi | \psi \rangle \equiv \delta_{\alpha\beta} \bar{Z}^\alpha Z^\beta \equiv \bar{Z}_\alpha Z^\alpha = 1 \quad [1]$$

where summation over repeated indices is understood, indices raised and lowered by $\delta^{\alpha\beta}$ and $\delta_{\alpha\beta}$, respectively, and the overbar refers to complex conjugation. A normalized state lies on the unit sphere $S \simeq S^{2n+1}$ in \mathbb{C}^{n+1} . Two nonzero states $|\psi\rangle$ and $|\varphi\rangle$ are equivalent, $|\psi\rangle \sim |\varphi\rangle$, iff they are related as $|\psi\rangle = \lambda |\varphi\rangle$ for some nonzero complex number λ . For equivalent states, physically meaningful quantities such as

$$\frac{\langle \psi | A | \psi \rangle}{\langle \psi | \psi \rangle}, \quad \frac{|\langle \psi | \varphi \rangle|^2}{\|\psi\|^2 \|\varphi\|^2} \quad [2]$$

(mean value of a physical quantity represented by a Hermitian operator A , transition probability from a physical state represented by $|\psi\rangle$ to one represented by $|\varphi\rangle$) are invariant. Hence, the real space of states representing the physical states of a quantum system unambiguously is the set of equivalence classes $\mathcal{P} \equiv \mathcal{H} / \sim$. \mathcal{P} is called the “space of rays.” For $\mathcal{H} \simeq \mathbb{C}^{n+1}$, we have $\mathcal{P} \simeq \mathbb{C}P^n$, where $\mathbb{C}P^n$ is the n -dimensional complex projective space. For normalized states, $|\psi\rangle$ and $|\varphi\rangle$ are equivalent iff $|\psi\rangle = \lambda |\varphi\rangle$, where $|\lambda| = 1$, that is, $\lambda \in U(1)$. Thus, two normalized states are equivalent iff they differ merely in a complex phase. It is well known that S can be regarded as the total space of a principal bundle over \mathcal{P} with structure group $U(1)$. This means that we have the projection

$$\pi : |\psi\rangle \in S \subset \mathcal{H} \rightarrow |\psi\rangle \langle \psi| \in \mathcal{P} \quad [3]$$

where the rank-1 projector $|\psi\rangle \langle \psi|$ represents the equivalence class of $|\psi\rangle$. Since we will use this bundle frequently in this article, we call it η_1 (the meaning of the subscript 1 will be clarified later). Then, we have

$$\eta_1 : U(1) \hookrightarrow S \xrightarrow{\pi} \mathcal{P} \quad [4]$$

For $Z^0 \neq 0$ the space of rays \mathcal{P} can be given local coordinates

$$w^j \equiv Z^j / Z^0, \quad j = 1, \dots, n \quad [5]$$

The w^j are inhomogeneous coordinates for CP^n on the coordinate patch \mathcal{U}_0 defined by the condition $Z^0 \neq 0$.

\mathcal{P} is a compact complex manifold with a natural Riemannian metric g . This metric g is induced from the scalar product on \mathcal{H} . Let us consider the construction of g by using the physical input provided by the invariance of the transition probability of [1]. For this we define a distance between $|\psi\rangle\langle\psi|$ and $|\varphi\rangle\langle\varphi|$ in \mathcal{P} as follows:

$$\cos^2(\delta(\psi, \varphi)/2) \equiv \frac{|\langle\psi|\varphi\rangle|^2}{\|\psi\|^2\|\varphi\|^2} \quad [6]$$

This definition makes sense since, due to the Cauchy-Schwartz inequality, the right-hand side of [6] is non-negative and ≤ 1 . It is equal to 1 iff $|\psi\rangle$ is a nonzero complex multiple of $|\varphi\rangle$, that is, iff they define the same point in \mathcal{P} . Hence in this case, $\delta(\psi, \varphi) = 0$ as expected.

Suppose now that $|\psi\rangle$ and $|\varphi\rangle$ are separated by an infinitesimal distance $ds \equiv \delta(\psi, \varphi)$. Putting this into the definition [6], using the local coordinates w^j of [5] for $|\psi\rangle$ and $w^j + dw^j$ for $|\varphi\rangle$ after expanding both sides using Taylor series, one gets

$$ds^2 = 4g_{j\bar{k}} dw^j d\bar{w}^{\bar{k}}, \quad j, \bar{k} = 1, 2, \dots, n \quad [7]$$

where

$$g_{j\bar{k}} \equiv \frac{(1 + \bar{w}_l w^l) \delta_{jk} - \bar{w}_j w_k}{(1 + \bar{w}_m w^m)^2} \quad [8]$$

with $dw^{\bar{k}} \equiv d\bar{w}^{\bar{k}}$. The line element [7] defines the Fubini-Study metric for \mathcal{P} .

The Pancharatnam Connection

Having defined the basic entity, the space of rays \mathcal{P} , and the principal $U(1)$ bundle η_1 , now we define a connection giving rise to a local law of parallel transport. This approach gives rise to a very general definition of the geometric phase. In the mathematical literature, the connection defined below is called the “canonical connection” on the principal bundle. However, since the motivation is coming from physics, we are going to rediscover this construction using merely physical information provided by quantum theory alone.

The information needed is an adaptation of Pancharatnam’s study of polarized light to quantum mechanics. Let us consider two normalized states $|\psi\rangle$ and $|\varphi\rangle$. When these states belong to the same ray, then we have $|\psi\rangle = e^{i\phi}|\varphi\rangle$ for some phase factor $e^{i\phi}$; hence, the phase difference between them can be defined to be just ϕ . How to define the phase difference between $|\psi\rangle$

and $|\varphi\rangle$ (not orthogonal) when these states belong to different rays? To compare the phases of nonorthogonal states belonging to different rays, Pancharatnam employed the following simple rule: two states are “in phase” iff their interference is maximal. In order to find the state $|\varphi\rangle \equiv e^{i\phi}|\varphi'\rangle$ from the ray spanned by the representative $|\varphi'\rangle$ which is “in phase” with $|\psi\rangle$, we have to find a ϕ modulo 2π for which the interference term in

$$\|\psi + e^{i\phi}\varphi'\|^2 = 2(1 + \text{Re}(e^{i\phi}\langle\psi|\varphi'\rangle)) \quad [9]$$

is maximal. Obviously the interference is maximal iff $e^{i\phi}\langle\psi|\varphi'\rangle$ is a real positive number, that is,

$$e^{i\phi} = \frac{\langle\varphi'|\psi\rangle}{|\langle\varphi'|\psi\rangle|}, \quad |\varphi\rangle = |\varphi'\rangle \frac{\langle\varphi'|\psi\rangle}{|\langle\varphi'|\psi\rangle|} \quad [10]$$

Hence for the state $|\varphi\rangle$ “in phase” with $|\psi\rangle$, one has

$$\langle\psi|\varphi\rangle = |\langle\psi|\varphi'\rangle| \in \mathbb{R}^+ \quad [11]$$

When such $|\psi\rangle$ and $|\varphi\rangle \equiv |\psi + d\psi\rangle$ are infinitesimally separated, from [11] it follows that

$$\text{Im}\langle\psi|d\psi\rangle = \frac{1}{2i}(\bar{Z}_\alpha dZ^\alpha - d\bar{Z}_\alpha Z^\alpha) = 0 \quad [12]$$

where $\bar{Z}_\alpha Z^\alpha = \bar{Z}_0 Z^0(1 + \bar{w}_j w^j) = 1$ due to normalization. Writing $Z^0 \equiv |Z^0|e^{i\Phi}$ using [5], one obtains

$$\text{Im}\langle\psi|d\psi\rangle = d\Phi + A = 0, \quad A \equiv \text{Im} \frac{\bar{w}_j dw^j}{1 + \bar{w}_k w^k} \quad [13]$$

In order to clarify the meaning of the 1-form A , notice that the choice

$$|\psi'\rangle \equiv \frac{1}{\sqrt{1 + \bar{w}_k w^k}} \begin{pmatrix} 1 \\ w^j \end{pmatrix} \quad [14]$$

defines a local section of the bundle η_1 . In terms of this section, the state $|\psi\rangle$ can be expressed as

$$|\psi\rangle = \begin{pmatrix} Z^0 \\ Z^j \end{pmatrix} = |Z^0|e^{i\Phi} \begin{pmatrix} 1 \\ w^j \end{pmatrix} = e^{i\Phi}|\psi'\rangle \quad [15]$$

For a path $w^j(t)$ lying entirely in $\mathcal{U}_0 \subset \mathcal{P}$, $|\psi(t)\rangle = e^{i\Phi(t)}|\psi'(t)\rangle$ defines a path in \mathcal{S} with a $\Phi(t)$ satisfying the equation $\dot{\Phi} + A = 0$. For a closed path C , the equation above defines a (generically) open path Γ projecting onto C by the projection π . It must be clear by now that the process described is the one of parallel transports with respect to a connection with a connection 1-form ω . The pull-back of ω with respect to the local section in [14] is the 1-form ($U(1)$ gauge field) A in [13]. The curve Γ corresponding to $|\psi(t)\rangle$ is the horizontal lift of C in \mathcal{P} . The $U(1)$ phase

$$e^{i\Phi[C]} \equiv e^{-i \oint_C A} \quad [16]$$

is the holonomy of the connection. We call this connection the “Pancharatnam connection,” and its holonomy for a closed path in the space of rays is the geometric phase acquired by the wave function. Now the question of fundamental importance is: how to realize closed paths in \mathcal{P} physically? This question is addressed in the following sections.

Quantum Jumps

We have seen that physical states of a quantum system are represented by the space of rays \mathcal{P} and normalized states used as representatives for such states form the total space \mathcal{S} of a principal $U(1)$ bundle η_1 over \mathcal{P} . Moreover, in the previous section we have realized that the physical notions of transition probability, and quantum interference naturally lead to the introduction of a Riemannian metric g and an abelian $U(1)$ gauge field A living on \mathcal{P} .

An interesting result based on the connection between g and A concerns a nice geometric description of a special type of quantum evolution consisting of a sequence of “quantum jumps.”

Consider two nonorthogonal rays $|A\rangle\langle A|$ and $|B\rangle\langle B|$ in \mathcal{P} . Let us suppose that the system’s normalized wave function initially is $|A\rangle \in \mathcal{S}$, and measure by the “polarizer” $|B\rangle\langle B|$. Then the result of this filtering measurement is $|B\rangle\langle B|A\rangle$, or after projecting back to the set of normalized states we have the “quantum jump”

$$|A\rangle \rightarrow |B\rangle \frac{\langle B|A\rangle}{|\langle B|A\rangle|} \quad [17]$$

Now we have the following theorem:

Theorem *The [17] jump can be recovered by parallel transporting the normalized state $|A\rangle$ according to the Pancharatnam connection along the shortest geodesic (with respect to the [8] metric), connecting $|A\rangle\langle A|$ and $|B\rangle\langle B|$ in \mathcal{P} .*

Let us now consider a cyclic series of filtering measurements with projectors $|A_a\rangle\langle A_a|$, $a=1,2,\dots,N+1$, where $|A_1\rangle\langle A_1| = |A_{N+1}\rangle\langle A_{N+1}|$. Prepare the system in the state $|A_1\rangle \in \mathcal{S}$, and then subject it to the sequence of filtering measurements. Then according to the theorem, the phase

$$e^{i\Phi} = \frac{\langle A_1|A_N\rangle\langle A_N|A_{N-1}\rangle\cdots\langle A_2|A_1\rangle}{|\langle A_1|A_N\rangle\langle A_N|A_{N-1}\rangle\cdots\langle A_2|A_1\rangle|} \quad [18]$$

picked up by the state is equal to the one obtained by parallel transporting $|A_1\rangle$ along a geodesic polygon consisting of the shorter arcs connecting

the projectors $|A_a\rangle\langle A_a|$ and $|A_{a+1}\rangle\langle A_{a+1}|$ with $a=1,2,\dots,N$. It is important to realize that this filtering measurement process is not a unitary one; hence, unitarity is not essential for the geometric phase to appear.

In this section we have managed to obtain closed paths in the form of geodesic polygons in \mathcal{P} via the physical process of subjecting the initial state $|A_1\rangle$ to a sequence of filtering measurements. It is clear that for any type of evolution, the geodesics of the Fubini-study metric play a fundamental role since any smooth closed curve in \mathcal{P} can be approximated by geodesic polygons.

Nonunitary evolution provided by the quantum measuring process is only half of the story. In the next section, we start describing closed paths in \mathcal{P} arising also from unitary evolutions generated by parameter-dependent Hamiltonians, the original context where geometric phases were discovered.

Unitary Evolutions

Adiabatic Evolution

Suppose that the evolution of our quantum system with $\mathcal{H} \simeq \mathbb{C}^{n+1}$ is generated by a Hermitian Hamiltonian matrix depending on a set of external parameters x^μ , $\mu=1,2,\dots,M$. Here we assume that the x^μ are local coordinates on some coordinate patch \mathcal{V} of a smooth M -dimensional manifold \mathcal{M} . We label the eigenvalues of $H(x)$ by the numbers $r=0,1,2,\dots,n$, and assume that the r th eigenvalue $E_r(x)$ is nondegenerate:

$$H(x)|r,x\rangle = E_r(x)|r,x\rangle, \quad r=0,1,2,\dots,n \quad [19]$$

We assume that $H(x)$, $E_r(x)$, $|r,x\rangle$ are smooth functions of x . The rank-1 spectral projectors

$$P_r(x) \equiv |r,x\rangle\langle r,x|, \quad r=0,1,2,\dots,n \quad [20]$$

for each r define a map $f_r: \mathcal{M} \rightarrow \mathcal{P}$:

$$f_r: x \in \mathcal{V} \subset \mathcal{M} \mapsto P_r(x) \in \mathcal{P} \quad [21]$$

Recall now that we have the bundle η_1 over \mathcal{P} , at our disposal, and we can pull back η_1 using the map f_r to construct a new bundle ξ_1^r over the parameter space \mathcal{M} . Moreover, we can define a connection on ξ_1^r by pulling back the canonical (Pancharatnam) connection of η_1 . The resulting bundle ξ_1^r is called the Berry–Simon bundle over the parameter space \mathcal{M} . Explicitly,

$$\xi_1^r: U(1) \hookrightarrow \xi_1^r \xrightarrow{\pi_\xi} \mathcal{M} \quad [22]$$

The states $|r,x\rangle$ of [19] define a local section of ξ_1^r . Suppressing the index r , the relationship between η_1

and ξ_1 can be summarized by the following diagram:

$$\begin{array}{ccc} \xi_1 & \xleftarrow{f^*} & \eta_1 \\ \pi_{\xi} \downarrow & & \downarrow \pi_{\eta} \\ \mathcal{M} & \xrightarrow{f} & \mathcal{P} \end{array} \quad [23]$$

Here f^* denotes the pullback map, and we have $\xi_1 \equiv f^*(\eta_1)$. (We have denoted the total space \mathcal{S} as η_1 .)

The local section of ξ_1 arising as the pullback of [14] an η_1 is given by

$$|r, x\rangle = \frac{1}{\sqrt{1 + \bar{w}^k(x)w_k(x)}} \begin{pmatrix} 1 \\ w^j(x) \end{pmatrix}, \quad x \in \mathcal{V} \subset \mathcal{M} \quad [24]$$

with $j=1, 2, \dots, n$. The pullback of the Pancharatanam connection ω on η_1 is $f^*(\omega)$. We can further pull back $f^*(\omega)$ to $\mathcal{V} \subset \mathcal{M}$ with respect to the local section of [24] to obtain a gauge field living on the parameter space. This gauge field is called the "Berry gauge field" and the corresponding connection is the Berry connection. Thus,

$$A = f^*(A) = A_{\mu}(x)dx^{\mu} = (A_j\partial_{\mu}w^j + A_{\bar{j}}\partial_{\mu}\bar{w}^{\bar{j}})dx^{\mu} \quad [25]$$

here $\partial_{\mu} \equiv \partial/\partial x^{\mu}$ and A is given by [13]. When we have a closed curve \mathcal{C} in \mathcal{M} , then $f \circ \mathcal{C}$ defines a closed curve \mathcal{C} in \mathcal{P} . We already know that the holonomy for \mathcal{C} in \mathcal{P} can be written in the [16] form; hence,

$$\Phi_B = - \oint_{f \circ \mathcal{C}} A = - \oint_{\mathcal{C}} f^*(A) = - \oint_{\mathcal{C}} A \quad [26]$$

This formula states that there is a geometric phase picked up by the eigenstates of a parameter-dependent Hermitian Hamiltonian when we change the parameters along a closed curve. Our formula shows that the geometric phase can be calculated using either the canonical connection on η_1 or the Berry connection on ξ_1 .

Let us then change the parameters x^{μ} adiabatically. The closed path in parameter space then defines Hamiltonians satisfying $H(x(T)) = H(x(0))$ for some $T \in \mathbb{R}^+$. Moreover, there is also the associated closed curve $P_r(x(T)) = P_r(x(0))$ in \mathcal{P} . The quantum adiabatic theorem states that if we prepare a state $|\Psi(0)\rangle \equiv |r, x(0)\rangle$ at $t=0$, which is an eigenstate of the instantaneous Hamiltonian $H(x(0))$, then after changing the parameters

infinitely slowly, the time evolution generated by the time-dependent Schrödinger equation

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = H(t) |\Psi(t)\rangle \quad [27]$$

takes the form

$$|\Psi(t)\rangle = |r, x(t)\rangle e^{i\Lambda_r(t)} \quad [28]$$

after time t , which belongs to the same eigensubspace. The point is that the theorem holds only for cases when the kinetic energy associated with the slow change in the external parameters is much smaller than the energy separation between $E_r(x)$ and $E_{r'}(x)$ for all $x \in \mathcal{M}$. Under this assumption, transitions between adjacent levels are prohibited during evolution. Notice that the adiabatic theorem clearly breaks down in the vicinity of level crossings where the gap is comparable with the magnitude of the kinetic energy of the external parameters.

However, if one takes it for granted that the projector $P_r(t) \equiv P_r(x(t))$ for some r satisfies the Schrödinger-von Neumann equation

$$i\hbar \frac{d}{dt} P_r(t) = [H(t), P_r(t)] \quad [29]$$

by virtue of [19], we get zero for the right-hand side. This means that $P_r(t)$ is constant; hence, the curve in \mathcal{P} degenerates to a point. The upshot of this is that exact adiabatic cyclic evolutions do not exist. It can be shown, however, that under certain conditions one can find an initial state $|\Psi(0)\rangle \neq |r, x(0)\rangle$ that is "close enough" to $P_r(x(t)) = |r, x(t)\rangle \langle r, x(t)|$. Then, we can say that the projector analog of [28] only approximately holds

$$|\Psi(t)\rangle \langle \Psi(t)| \simeq |r, x(t)\rangle \langle r, x(t)| \quad [30]$$

This means that the use of the bundle picture for the generation of closed curves for \mathcal{P} via the adiabatic evolution can merely be used as an approximation.

Berry's Phase

The straightforward calculation after substituting [28] into [27] shows that

$$\exp(i\Lambda_r(T)) \exp\left(-\frac{i}{\hbar} \int_0^T E_r(t) dt\right) \exp\left(-i \oint_{\mathcal{C}} \mathcal{A}^{(r)}\right) \quad [31]$$

where \mathcal{C} is a closed curve lying entirely in $\mathcal{V} \subset \mathcal{M}$. The first phase factor is the dynamical and the second is the celebrated Berry phase. Notice that the index r labeling the eigensubspace in question

should now be included in the definition of \mathcal{A} (see eqn [25]).

As an explicit example, let us take the Hamiltonian

$$H(\mathbf{X}(t)) = -\omega_0 \mathbf{J} \cdot \mathbf{X}(t), \quad \omega_0 \equiv \frac{Bge}{2mc},$$

$$\mathbf{X} \in \mathbb{R}^3, \quad |\mathbf{X}| = 1 \quad [32]$$

where e , m , and g are the charge, mass, and Landé factor of a particle, c is the speed of light, and B is the (constant) magnitude of an applied magnetic field. The three components of \mathbf{J} are $(2J+1) \times (2J+1)$ -dimensional spin matrices satisfying $\mathbf{J} \times \mathbf{J} = i\hbar \mathbf{J}$. The Hamiltonian (eqn [32]) describes a spin J particle moving in a magnetic field with slowly varying direction. It is obvious that the parameter space is a 2-sphere. Introducing polar coordinates $0 \leq \theta < \pi$, $0 \leq \chi < 2\pi$ for the patch \mathcal{V} of S^2 excluding the south pole, we have $x^1 \equiv \theta$, $x^2 \equiv \chi$.

As an illustration, let us consider the spin 1/2 case. Then H can be expressed in terms of the 2×2 Pauli matrices. The eigenvalues are $E_0 = -\omega_0 \hbar/2$ and $E_1 = \omega_0 \hbar/2$ ($r=0,1$). For the ground state, the mapping f_0 of [21] from $\mathcal{V} \subset \mathcal{M} \simeq S^2$ to $\mathcal{P} \simeq \mathbb{CP}^1$ is given by

$$w(\theta, \chi) \equiv \tan\left(\frac{\theta}{2}\right) e^{i\chi} \quad [33]$$

which is stereographic projection of S^2 from the south pole onto the complex plane corresponding to the coordinate patch $\mathcal{U}_0 \subset \mathbb{CP}^1$. Using [13] and [25], one can calculate the pullback gauge field and its curvature $\mathcal{F}^{(0)} \equiv d\mathcal{A}^{(0)}$, where

$$\mathcal{A}^{(0)} = \frac{1}{2}(1 - \cos\theta)d\chi, \quad \mathcal{F}^{(0)} = \frac{1}{2}\sin\theta d\theta \wedge d\chi \quad [34]$$

Notice that $\mathcal{F}^{(0)}$ is the field strength of a magnetic monopole of strength 1/2 living on \mathcal{M} . Using Stokes theorem, from [26] one can calculate Berry's phase

$$\Phi^{(0)}[C] = -\oint_C \mathcal{A}^{(0)} = -\int_S \mathcal{F}^{(0)} = -\frac{1}{2}\Omega[C] \quad [35]$$

where S is the surface bounded by the loop C and $\Omega[C]$ is the solid angle subtended by the curve C at $\mathbf{X} = 0$.

The above result can be generalized for arbitrary spin J . Then, we have the eigenvalues $E_r = -\omega_0 \hbar(J-r)$, where $0 \leq r \leq 2J$. The final result in this case is

$$\Phi^{(r)}[C] = -(J-r)\Omega[C], \quad 0 \leq r \leq 2J \quad [36]$$

The Aharonov–Anandan Phase

We have seen that the quantum adiabatic theorem can only be used approximately for generating

closed curves in \mathcal{P} . This section, describes as to how such curves can be generated exactly.

Let us consider the Schrödinger equation with a time-dependent Hamiltonian (eqn [27]). Then we call its solution $|\Psi(t)\rangle$ cyclic if the state of the system returns, after a period T , to its original state. This means that the projector $|\Psi(t)\rangle\langle\Psi(t)|$ traverses a closed path C in \mathcal{P} . In order to realize this situation, we have to find solutions of [27] for which $|\Psi(T)\rangle = e^{i\Delta_\Psi} |\Psi(0)\rangle$ for some Δ_Ψ .

Taking for granted the existence of such a solution, let us first explore its consequences. First, we remove the dynamical phase from the cyclic solution $|\Psi(t)\rangle$

$$|\psi(t)\rangle \equiv \exp\left(\frac{i}{\hbar} \int_0^t \langle\Psi(t')|H(t')|\Psi(t')\rangle dt'\right) |\Psi(t)\rangle \quad [37]$$

Then, $|\psi(t)\rangle$ satisfies [12], that is, it defines a unique horizontal lift of the closed curve C in \mathcal{P} . Following the same steps as in section describing the Pancharatanam condition, we see that the phase

$$\Phi_{AA}[C] = -\oint_C A$$

$$= \Delta_\Psi + \frac{1}{\hbar} \int_0^T \langle\Psi(t)|H(t)|\Psi(t)\rangle dt \quad [38]$$

is purely geometric in origin. It is called the Aharonov–Anandan (AA) phase.

Let us now turn back to the question of finding cyclic states satisfying $|\Psi(T)\rangle = e^{i\Delta_\Psi} |\Psi(0)\rangle$. One possible solution is as follows. Suppose that H depends on time through some not necessarily slowly changing parameters x . Let us find a partner Hamiltonian h for our H by defining a smooth mapping $\sigma: \mathcal{M} \rightarrow \mathcal{M}$, such that

$$h(x) \equiv H(\sigma(x)), \quad x \in \mathcal{V} \subset \mathcal{M} \quad [39]$$

For the special class we study here, the cyclic vectors are eigenvectors of $h(x)$. Hence, the projectors p_r and P_r of h and H are related as $p_r(x) = P_r(\sigma(x))$; this means that we have a map $g_r: \mathcal{M} \rightarrow \mathcal{P}$,

$$g_r \equiv f_r \circ \sigma: x \in \mathcal{V} \subset \mathcal{M} \rightarrow p_r(x) \in \mathcal{P} \quad [40]$$

which associates with every x an eigenstate of $h(x)$. Moreover, g_r associates with a closed curve C in \mathcal{M} a closed curve C in \mathcal{P} . Notice that generically $[h(x), H(x)] \neq 0$; hence, cyclic states are not eigenstates of the instantaneous Hamiltonian.

It should be clear by now that we can repeat the construction as discussed in the adiabatic case with g_r replacing f_r . In particular, we can construct a new bundle ζ_1 over the parameter space via the usual

pullback procedure. More precisely, we have the corresponding diagram

$$\begin{array}{ccc} \zeta_1 & \xleftarrow{g^*} & \eta_1 \\ \pi_\zeta \downarrow & & \downarrow \pi_\eta \\ \mathcal{M} & \xrightarrow{g} & \mathcal{P} \end{array} \quad [41]$$

The AA connection can be obtained by pulling back the Pancharatnam connection:

$$a \equiv g^*(A) = \sigma^* \circ f^*(A) = \sigma^*(A) \quad [42]$$

where the last equality relates the AA connection with the Berry connection. Now the AA phase is

$$\Phi_{AA} = - \oint_{g \circ \mathcal{C}} A = - \oint_{\mathcal{C}} g^*(A) = - \oint_{\mathcal{C}} a \quad [43]$$

As an example, let us take the Hamiltonian [32] with the curve \mathcal{C} on $\mathcal{M} \equiv S^2$:

$$X(t) = (\sin \theta \cos(\chi + \omega t), \sin \theta \sin(\chi + \omega t), \cos \theta) \quad [44]$$

Here θ and χ are the polar coordinates of a fixed point in S^2 where the motion starts. The curve \mathcal{C} is a circle of fixed latitude and is traversed with an arbitrary speed. This model can be solved exactly and it can be shown that the mapping $\sigma_s: S^2 \rightarrow S^2$ is given by

$$\begin{aligned} \sigma : (u, \chi) &\mapsto \left(\frac{u - s}{\sqrt{s^2 - 2us + 1}}, \chi \right), \\ u &\equiv \cos \theta, \quad s \equiv \frac{\omega}{\omega_0} \end{aligned} \quad [45]$$

One can prove that for $0 \leq s < 1$, σ_s is a diffeomorphism. In the $s \rightarrow 0$ (the adiabatic) limit, the mapping $g_{r,s} \equiv f_{r,s} \circ \sigma_s$ is continuously deformed to f_r . Moreover, $h(x)$ as defined above commutes with the time evolution operator; hence, cyclic states are indeed eigenstates of $h(x)$.

Using [42], [43], and [45], the explicit form of σ_s , we get for the AA phase

$$\Phi_{AA}^{(r,s)}[\mathcal{C}] = -2\pi(J - r) \left(1 - \frac{u - s}{\sqrt{s^2 - 2us + 1}} \right) \quad [46]$$

In the adiabatic limit, the result goes to $-2\pi(J - r)(1 - u)$ which is just $-(J - r)$ times the solid angle of the path of fixed latitude, as it has to be.

Generalization

In the sequence of examples, we have shown that geometric phases are related to the geometric structures on the bundle η_1 . The Berry and AA phases are special cases arising from Pancharatnam's phase via a pullback procedure with respect to suitable maps

defined by the physical situation in question. Hence, the Pancharatnam connection in this sense is universal. The root of this universality rests in a deep theorem of mathematics concerning the existence of universal bundles and their universal connections. In order to elaborate the insight provided by this theorem into the geometry of quantum evolution, let us first make a further generalization.

In our study of time-dependent Hamiltonians we have assumed that the eigenvalues of [19] were nondegenerate. Let us now relax this assumption. Fix an integer $N \geq 1$, the degeneracy of the eigensubspace corresponding to the eigenvalue E_r . One can then form a $U(N)$ principal bundle ξ_N over \mathcal{M} , furnished with a connection, that is a natural generalization of the Berry connection. The pullback of this connection to a patch of \mathcal{M} is a $U(N)$ -valued gauge field and its holonomy along a loop in \mathcal{M} gives rise to a $U(N)$ matrix generalization of the $U(1)$ Berry phase.

The natural description of this connection and its AA analog is as follows. Take the complex Grassmannian $Gr(n+1, N)$ of N planes in \mathbb{C}^{n+1} . Obviously, $Gr(n+1, 1) \equiv \mathcal{P}$. Each point of $Gr(n+1, N)$ corresponds to an N plane through the origin represented by a rank- N projector. This projector can be written in terms of N orthonormal basis vectors in an infinite number of ways. This ambiguity of choosing orthonormal frames is captured by the $U(N)$ gauge symmetry, the analog of the $U(1)$ (phase) ambiguity in defining a normalized state as the representative of the rank-1 projector. This bundle of frames is the Stiefel bundle $V(n+1, N)$ alternatively denoted by η_N . $V(n+1, N)$ is a principal $U(N)$ bundle over $Gr(n+1, N)$ equipped with a canonical connection ω_N which is the $U(N)$ analog of Pancharatnam's connection.

Now according to the powerful theorem of Narasimhan and Ramanan if we have a $U(N)$ bundle ξ_N over the M -dimensional parameter space \mathcal{M} , then there exists an integer $n_0(N, M)$ such that for $n \leq n_0$ there exists a map $f: \mathcal{M} \rightarrow Gr(n+1, N)$ such that $\eta_N = f^*(V(n+1, N))$. Moreover, given any two such maps f and g , the corresponding pullback bundles are isomorphic if and only if f is homotopic to g .

For the examples of the sections "Berry's phase" and "The Aharonov-Anandan phase," we have $N=1, n=1$, and $M=2$. Since the maps f_r and $g_{r,s}$ defined by the rank-1 spectral projectors of $H(x)$ and $h(x)$ for $0 \leq s < 1$ are homotopic, the corresponding pullback bundles ξ_1 and ζ_1 are isomorphic. Moreover, the Berry and AA connections are the pullbacks of the universal connection on $V(n+1, 1) \equiv \eta_1$ which is just Pancharatnam's connection.

For the infinite-dimensional case, one can define $Gr(\infty, N)$ by taking the union of the natural inclusion maps of $Gr(n, N)$ into $Gr(n+1, N)$.

We denote this universal classifying bundle $V(\infty, N)$ as η . Then, we see that given an N -dimensional eigensubspace bundle over \mathcal{M} and a map $f_r: x \in \mathcal{M} \mapsto P_r(x) \in Gr(\infty, N)$ defined by the physical situation, the geometry of evolving eigensubspaces can be understood in terms of the holonomy of the pullback of the universal connection on η .

Conclusions

In this article, we elucidate the mathematical origin of geometric phases. We have seen that the key observation is the fact that the space of rays \mathcal{P} represents unambiguously the physical states of a quantum system. The particular representatives of a class in \mathcal{P} belonging to the usual Hilbert space \mathcal{H} form (local) sections of a $U(1)$ bundle η_1 . Based on the physical notions of transition probability and interference, η_1 can be furnished with extra structures: the metric and the connection, the latter giving rise to a natural definition of parallel transport. We have seen that the geodesics of \mathcal{P} with respect to the metric play a fundamental role in approximating evolutions of any kind, giving rise to a curve in \mathcal{P} .

The geometric structures of η_1 induce similar structures for pullback bundles. These bundles encapsulate the geometric details of time evolutions generated by Hamiltonians that depend on a set of parameters x belonging to a manifold \mathcal{M} . It was shown that the famous examples of Berry and AA phases arise as an important special case in this formalism. A generalization of evolving N -dimensional subspaces based on the theory of universal connections can also be given. This shows that the basic structure responsible for the occurrence of anholonomy effects in evolving quantum systems is the universal bundle η which is the bundle of subspaces of arbitrary dimension N in a Hilbert space.

The important issue of applying the idea of anholonomy to physical problems has not been

dealt with in this article. There are spectacular applications such as holonomic quantum computation, the gauge kinematics of deformable bodies, quantum Hall-effect, fractional spin and statistics. The interested reader should consult the vast literature on the subject or as a first glance, the book of Shapere and Wilczek (1989).

See also: Fractional Quantum Hall Effect; Geometric Measure Theory; Holomorphic Dynamics; Moduli Spaces: An Introduction.

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Geophysical Dynamics

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Introduction

The equations of geophysical fluid dynamics are the equations governing the motion of the atmosphere and the ocean, and are derived from the conservation equations from physics, namely conservation of mass,

momentum, energy, and some other components such as salt for the ocean, humidity (or chemical pollutants) for the atmosphere.

The first assumption used in any circulation model is the well-accepted Boussinesq approximation, that is, the density differences are neglected in the system except in the buoyancy term and in the equation of state. The resulting system is the so-called Boussinesq equations (Pedlosky 1987). Due to the extremely high accuracy of this approximation, these equations are considered as the basic equations

in geophysical dynamics. From the computational point of view, however, the Boussinesq equations are still not accessible.

Owing to the difference of sizes of the vertical and horizontal dimensions, both in the atmosphere and in the ocean (10–20 km versus several thousands of kilometers), the second approximation is based on the smallness of the vertical length scales with respect to the horizontal length scales, that is, oceans (and the atmosphere) compose very thin layers. The scale analysis ensures that the dominant forces in the vertical-momentum equation come from the pressure gradient and the gravity. This leads to the so-called hydrostatic approximation, which amounts to replacing the vertical component of the momentum equation by the hydrostatic balance equation, and hence leading to the well-accepted primitive equations (PEs) (Washington and Parkinson 1986). As far as we know, the primitive equations were first considered by L F Richardson (1922); when it appeared that they were still too complicated they were left out and, instead, attention was focused on even simpler models, the geostrophic and quasigeostrophic models, considered in the late 1940s by J von Neumann and his collaborators, in particular J G Charney. With the increase of computing power, interest eventually returned to the PEs, which are now the core of many global circulation models (GCMs) or ocean global circulation models (OGCMs), available at the National Center for Atmospheric Research (NCAR) and elsewhere. GCMs and OGCMs are very complex models which contain many components, but still, the PEs are the central component for the dynamics of the air or the water. Further approximations based on the fast rotation of the Earth implying the smallness of the Rossby number lead to the quasigeostrophic and geostrophic equations (Pedlosky 1987).

The mathematical study of the PEs was initiated by Lions, Teman, and Wang in the early 1990s. They produced a mathematical formulation of the PEs which resembles that of the Navier–Stokes due to Leray, and obtained the existence, for all time, of weak solutions (see Lions *et al.* 1992a, b, 1993, 1995). Further works conducted during the 1990s have improved and supplemented these early results bringing the mathematical theory of the PEs to that of the three-dimensional incompressible Navier–Stokes equations (Constantin and Foias 1998, Teman 2001). In summary, the following results are now available which will be presented in this article:

1. existence of weak solutions for all time;
2. existence of strong solutions in space dimension three, local in time;
3. existence and uniqueness of a strong solution in space dimension two, for all time; and

4. uniqueness of weak solutions in space dimension two.

The PEs of the Ocean

The ocean is made up of a slightly compressible fluid subject to a Coriolis force. The full set of equations of the large-scale ocean are the following: the conservation of momentum equation, the continuity equation (conservation of mass), the thermodynamics equation, the equation of state and the equation of diffusion for the salinity S :

$$\rho \frac{dV_3}{dt} + 2\rho \Omega \times V_3 + \nabla_3 p + \rho g = D \quad [1]$$

$$\frac{d\rho}{dt} + \rho \operatorname{div}_3 V_3 = 0 \quad [2]$$

$$\frac{dT}{dt} = Q_T \quad [3]$$

$$\frac{dS}{dt} = Q_S \quad [4]$$

$$\rho = f(T, S, p) \quad [5]$$

Here V_3 is the three-dimensional velocity vector, $V_3 = (u, v, w)$, ρ , p , T are respectively, the density, pressure, and temperature, and S is the concentration of salinity; $g = (0, 0, g)$ is the gravity vector, D the molecular dissipation, Q_T and Q_S are the heat and salinity diffusions, respectively.

Remark 1 The equation of state for the oceans is derived on a phenomenological basis. Only empirical forms of the function $f(T, S, \rho)$ are known (see Washington and Parkinson (1986)). It is natural, however, to expect that ρ decreases if T increases and that ρ increases if S increases. The simplest law is

$$\rho = \rho_0(1 - \beta_T(T - T_r) + \beta_S(S - S_r)) \quad [6]$$

corresponding to a linearization around reference values ρ_0 , T_r , S_r of respectively, the density, temperature, and the salinity, β_T and β_S are positive expansion coefficients.

The Mach number for the flow in the ocean is not large and, therefore, as a starting point, we can make the so-called Boussinesq approximation in which the density is assumed constant, $\rho = \rho_0$, except in the buoyancy term and in the equation of state. This amounts to replacing [1], [2] by

$$\rho_0 \frac{dV_3}{dt} + 2\rho_0 \Omega \times V_3 + \nabla_3 p + \rho g = D \quad [7]$$

$$\operatorname{div}_3 V_3 = 0 \quad [8]$$

Furthermore, since for large-scale ocean, the horizontal scale is much larger than the vertical one, a scale analysis (Pedlosky 1987) shows that $\partial p / \partial z$ and ρg are

the dominant terms in the vertical-momentum equation, leading to the hydrostatic approximation

$$\frac{\partial p}{\partial z} = -\rho g \quad [9]$$

For mid-latitude regional studies, it is usual to consider the beta-plane approximation of the equations. Thus, we assume that the ocean fills a domain \mathcal{M}_ε of \mathbb{R}^3 . The top of the ocean is a domain Γ_i included in the surface of the earth S_a (sphere of radius a centered at 0). The bottom Γ_b of the ocean is defined by $(z = x_3 = r - a)$, $z = -\varepsilon h(\theta, \varphi)$, where $\varepsilon > 0$ is a positive parameter. It is introduced to take into consideration the smallness of the vertical scales compared to the horizontal scales. h is a function of class \mathcal{C}^2 at least on $\bar{\Gamma}_i$; it is assumed also that h is bounded from below, that is, $0 < \underline{h} \leq h(\theta, \varphi) \leq \bar{h}$, $(\theta, \varphi) \in \Gamma_i$. The lateral surface Γ_l consists of the part of cylinder $\{(\theta, \varphi) \in \partial\Gamma_i, -\varepsilon h(\theta, \varphi) \leq r \leq 0\}$. The PEs of the ocean are given by

$$\begin{aligned} \frac{\partial \mathbf{v}}{\partial t} + \nabla_\nu \mathbf{v} + w \frac{\partial \mathbf{v}}{\partial z} + \frac{1}{\rho_0} \nabla p \\ + 2\Omega \sin \theta \mathbf{k} \times \mathbf{v} - \mu_\nu \Delta \mathbf{v} - \nu_\nu \frac{\partial^2 \mathbf{v}}{\partial z^2} = F_\nu \end{aligned} \quad [10]$$

$$\frac{\partial p}{\partial z} = -\rho, \quad \operatorname{div} \mathbf{v} + \frac{\partial w}{\partial z} = 0 \quad [11]$$

$$\frac{\partial T}{\partial t} + \nabla_\nu T + w \frac{\partial T}{\partial z} - \mu_T \Delta T - \nu_T \frac{\partial^2 T}{\partial z^2} = F_T \quad [12]$$

$$\frac{\partial S}{\partial t} + \nabla_\nu S + w \frac{\partial S}{\partial z} - \mu_S \Delta S - \nu_S \frac{\partial^2 S}{\partial z^2} = F_S \quad [13]$$

$$\operatorname{div} \int_{-h}^0 \mathbf{v} dz = 0 \quad [14]$$

$$p = p_s + P, \quad P = P(T, S) = g \int_z^0 p dz' \quad [15]$$

$$\rho = \rho_0(1 - \beta_T(T - T_r) + \beta_S(S - S_r)) \quad [16]$$

$$\int_{\mathcal{M}_\varepsilon} S d\mathcal{M}_\varepsilon = 0 \quad [17]$$

where \mathbf{v} is the horizontal velocity of the water, w is the vertical velocity, and T_r, S_r are averaged (or reference) values of T and S . The diffusion coefficients μ_ν, μ_T, μ_S and ν_ν, ν_T, ν_S are different in the horizontal and vertical directions, accounting for some eddy diffusions in the sense of Smagorinsky (1962). Note that F_ν, F_T , and F_S correspond to volumic sources of horizontal momentum, heat, and salt, respectively.

Boundary conditions

There are several sets of natural boundary conditions that one can associate to the PEs; for instance, the following:

On the top of the ocean $\Gamma_i(z=0)$

$$\begin{aligned} \nu_\nu \frac{\partial \mathbf{v}}{\partial z} + \alpha_\nu(\mathbf{v} - \mathbf{v}_a) = \tau_\nu, \quad w = 0 \\ \nu_T \frac{\partial T}{\partial z} + \alpha_T(T - T_a) = 0, \quad \frac{\partial S}{\partial z} = 0 \end{aligned} \quad [18]$$

At the bottom of the ocean $\Gamma_b(z=-h(\theta, \varphi))$

$$\mathbf{v} = 0, \quad w = 0, \quad \frac{\partial T}{\partial \mathbf{n}_T} = 0, \quad \frac{\partial S}{\partial \mathbf{n}_S} = 0 \quad [19]$$

On the lateral boundary $\Gamma_l = \{-h(\theta, \varphi) < z < 0, (\theta, \varphi) \in \partial\Gamma_i\}$

$$\mathbf{v} = 0, \quad w = 0, \quad \frac{\partial T}{\partial \mathbf{n}_T} = 0, \quad \frac{\partial S}{\partial \mathbf{n}_S} = 0 \quad [20]$$

Here $\mathbf{n} = (n_H, n_z)$ is the unit outward normal on $\partial\mathcal{M}_\varepsilon$ decomposed into its horizontal and vertical components; the conormal derivatives $\partial/\partial \mathbf{n}_T$ and $\partial/\partial \mathbf{n}_S$ are those associated with the linear (temperature and salinity) operators,

$$\begin{aligned} \frac{\partial}{\partial \mathbf{n}_T} &= \mu_T n_H \cdot \nabla + \nu_T n_z \frac{\partial}{\partial z} \\ \frac{\partial}{\partial \mathbf{n}_S} &= \mu_S n_H \cdot \nabla + \nu_S n_z \frac{\partial}{\partial z} \end{aligned} \quad [21]$$

Equations [10]–[17] with boundary conditions [18]–[20] are supplemented with the initial conditions

$$\mathbf{v}|_{t=0} = \mathbf{v}_0, \quad T|_{t=0} = T_0, \quad S|_{t=0} = S_0 \quad [22]$$

where \mathbf{v}_0, T_0, S_0 are given initial data.

Following the work of Lions *et al.* (1992a, b, 1993, 1995) (see also Temam and Ziane (2004)), we introduce the following function spaces $V = V_1 \times V_2 \times V_3$, $H = H_1 \times H_2 \times H_3$, where

$$V_1 = \left\{ \mathbf{v} \in H^1(\mathcal{M})^2, \operatorname{div} \int_{-h}^0 \mathbf{v} dz = 0, \right. \\ \left. \mathbf{v} = 0 \text{ on } \Gamma_b \cup \Gamma_l \right\}$$

$$V_2 = H^1(\mathcal{M})$$

$$V_3 = \dot{H}^1(\mathcal{M}) = \left\{ S \in H^1(\mathcal{M}), \int_{\mathcal{M}} S d\mathcal{M} = 0 \right\}$$

$$H_1 = \left\{ \mathbf{v} \in L^2(\mathcal{M})^2, \operatorname{div} \int_{-h}^0 \mathbf{v} dz = 0, \right.$$

$$\left. n_H \cdot \int_{-h}^0 \mathbf{v} dz = 0 \text{ on } \partial\Gamma_i \text{ (i.e., on } \Gamma_l) \right\}$$

$$H_2 = L^2(\mathcal{M})$$

$$H_3 = \dot{L}^2(\mathcal{M}) = \left\{ S \in L^2(\mathcal{M}), \int_{\mathcal{M}} S d\mathcal{M} = 0 \right\}$$

The global existence of weak solutions is established in Lions *et al.* (1992b), using the Galerkin method and assuming the H^2 -regularity of the GFD–Stokes problem, which was established in Ziane

(1995). A more general global existence result based on the method of finite differences in time and independent of the H^2 -regularity is established in Temam and Ziane (2004), which we state here.

Theorem 2 *Given $t_1 > 0$, U_0 in H , and $F = (F_v, F_T, F_S)$ in $L^2(0, t_1; H)$; $g = g_v, g_T$ is given in $L^2(0, t_1; (L^2(\Gamma_i)^3))$. Then there exists*

$$U \in L^\infty(0, t_1; H) \cap L^2(0, t_1; V) \quad [23]$$

which is a weak solution of [10]–[17] and [18]–[20], [22]; furthermore, U is weakly continuous from $[0, t_1]$ into H .

Strong Solutions

The local existence and uniqueness of strong solutions of the primitive equations of the ocean relies on the H^2 -regularity of the stationary linear primitive equations associated to [10]–[17]:

$$\frac{1}{\rho_0} \nabla p + 2\Omega \sin \theta \mathbf{k} \times \mathbf{v} - \mu_v \Delta \mathbf{v} - \nu_v \frac{\partial^2 \mathbf{v}}{\partial z^2} = F_v \quad [24]$$

$$\int_{-h}^0 \operatorname{div} \mathbf{v} \, dz = 0$$

$$-\mu_T \Delta T - \nu_T \frac{\partial^2 T}{\partial z^2} = F_T \quad [25]$$

$$-\mu_S \Delta S - \nu_S \frac{\partial^2 S}{\partial z^2} = F_S$$

$$p = p_s + P, \quad P = P(T, S) = g \int_z^0 p \, dz' \quad [26]$$

with boundary conditions [18]–[20]. Here F_v, F_T, F_S are independent of time. We have the following H^2 -regularity of solutions (Ziane 1995, Hu *et al.* 2002, Temam and Ziane 2004).

Theorem 3 *Assume that h is in $C^4(\bar{\Gamma}_i)$, $h \geq \underline{h} > 0$, $F_v, F_T, F_S \in (L^2(\mathcal{M}_\varepsilon))^4$ and $g_v = \tau_v + \alpha_v \mathbf{v}_a$, $g_T = \alpha_a T_a \in (H_0^1(\Gamma_i))^4$. Let $(v, T, S; p) \in (H^1(\mathcal{M}_\varepsilon))^4 \times L^2(\Gamma_i)$ be a weak solution of [24]–[26]. Then*

$$(v, p) \in (H^2(\mathcal{M}_\varepsilon))^2 \times H^1(\mathcal{M}_\varepsilon) \quad [27]$$

$$(T, S) \in (H^2(\mathcal{M}_\varepsilon))^2$$

Moreover, the following inequalities hold:

$$|v|_{H^2(\mathcal{M}_\varepsilon)}^2 + \varepsilon |p|_{H^1(\Gamma_i)}^2 \leq C \left[|F_v|_\varepsilon^2 + |g_v|_{L^2(\Gamma_i)}^2 + \varepsilon |\nabla g_v|_{L^2(\Gamma_i)}^2 \right]$$

$$|T|_{H^2(\mathcal{M}_\varepsilon)}^2 \leq C \left[|F_T|^2 + |g_T|_{L^2(\Gamma_i)}^2 + \varepsilon |\nabla g_T|_{L^2(\Gamma_i)}^2 \right]$$

$$|S|_{H^2(\mathcal{M}_\varepsilon)}^2 \leq C |F_S|^2$$

where C is a positive constant independent of ε .

We now turn our attention to the nonlinear time-dependent PEs. The local-in-time existence and uniqueness of strong solutions is obtained in Temam and Ziane (2004); see also Hu *et al.* (2003) and Guillén-González *et al.* (2001). The proof is more involved than that of the three-dimensional Navier–Stokes equations. It consists of several steps. In the first step, one proves the global existence of strong solutions to the linearized time-dependent problem. In the second step, one uses the solution of the linearized equation in order to reduce the PEs to a nonlinear evolution equation with zero initial data and homogeneous boundary conditions. Finally, in the last step, one uses nonisotropic Sobolev inequalities together with Theorem 3. The local existence result is given by the following:

Theorem 4 *Let $\varepsilon > 0$ be given. We assume that Γ_i is of class C^3 and that $h: \bar{\Gamma}_i \rightarrow \mathbb{R}_+$ is of class C^3 . We are given U_0 in V , $F = (F_v, F_T, F_S)$ in $L^2(0, t_1; H)$ with $\partial F / \partial t$ in $L^2(0, t_1; L^2(\mathcal{M}_\varepsilon)^4)$, and $g = (g_v, g_T)$ in $L^2(0, t_1; H_0^1(\Gamma_i)^3)$ with $\partial g / \partial t$ in $L^2(0, t_1; H_0^1(\Gamma_i)^3)$. Then there exists $t_* > 0$, $t_* = t_*(\|U_0\|)$, and there exists a unique solution $U = U(t) = (v(t), T(t), S(t))$ of the PEs [10]–[17], [18]–[20], and [22] such that*

$$U \in C([0, t_*]; V) \cap L^2(0, t_*, H^2(\mathcal{M}_\varepsilon)^4) \quad [28]$$

The PEs of the Atmosphere

In this section we briefly describe the PEs of the atmosphere, for which all the mathematical results obtained for the PEs of the ocean are valid. We start from the conservations equations similar to [1]–[5]; in fact [1] and [2] are the same; the equation of energy conservation (temperature) is slightly different from [3] because of the compressibility of air; the state equation is that of perfect gas instead of [5]; finally, instead of the concentration of salt in the water, we consider the amount of water in air, q . Hence, we have

$$\rho \frac{dV_3}{dt} + 2\rho \Omega \times V_3 + \nabla_3 p + \rho g = D \quad [29]$$

$$\frac{d\rho}{dt} + \rho \operatorname{div}_3 V_3 = 0 \quad [30]$$

$$h c_p \frac{dT}{dt} - \frac{RT}{p} \frac{dp}{dt} = Q_T \quad [31]$$

$$\frac{dq}{dt} = 0, \quad p = R p T$$

Here $c_p > 0$ is the specific heat of air at constant pressure, and R is the specific gas constant for the air. Proceeding as in the PEs of the ocean, we decompose V_3 into its horizontal and vertical components, $V_3 = v + w$; then we use the hydrostatic approximation, replacing the equation of

conservation of vertical momentum by the hydrostatic equation [9]. We find

$$\frac{\partial v}{\partial t} + \nabla_v v + w \frac{\partial v}{\partial z} + \frac{1}{\nabla \rho_0} p + 2\Omega \sin \theta \times v - \mu_v \Delta v - \nu_v \frac{\partial^2 v}{\partial z^2} = 0 \quad [32]$$

$$\frac{\partial p}{\partial z} = -\rho g \quad [33]$$

$$\frac{\partial T}{\partial t} + \nabla_v T + w \frac{\partial T}{\partial z} - \mu_T \Delta T - \nu_T \frac{\partial^2 T}{\partial z^2} - \frac{RT}{p} \frac{dp}{dt} = Q_T \quad [34]$$

$$\frac{\partial q}{\partial t} + \nabla_v q + w \frac{\partial q}{\partial z} - \mu_q \Delta q - \nu_q \frac{\partial^2 q}{\partial z^2} = 0 \quad [35]$$

$$p = R\rho T \quad [36]$$

The right-hand side of [34], represents the solar heating.

Change of Vertical Coordinate

Since ρ does not vanish, the hydrostatic equation [33] implies that p is a strictly decreasing function of z , and we are thus allowed to use p as the vertical coordinate; hence in spherical geometry the independent variables are now φ, θ, p , and t . By an abuse of notation, we still denote by v, p, T, q, ρ these functions expressed in the φ, θ, p, t variables. We denote by w the vertical component of the wind in the new variables, and one can show that the PEs of the atmosphere become

$$\frac{\partial v}{\partial t} + \nabla_v v + w \frac{\partial v}{\partial p} + 2\Omega \sin \theta k \times v + \nabla \Phi - L_v v = F_v \quad [37]$$

$$\frac{\partial \Phi}{\partial p} + \frac{R}{p} T = 0 \quad [38]$$

$$\operatorname{div} v + \frac{\partial w}{\partial p} z = 0 \quad [39]$$

$$\frac{\partial T}{\partial t} + \nabla_v T + w \frac{\partial T}{\partial p} - \frac{RT}{p} \omega - L_T T = F_T \quad [40]$$

$$\frac{\partial q}{\partial t} + \nabla_v q + w \frac{\partial q}{\partial p} - L_q q = F_q \quad [41]$$

$$p = R\rho T \quad [42]$$

We have denoted by $\Phi = gz$ the geopotential (z is now function of φ, θ, p, t); L_v, L_T, L_q are the Laplace

operators, with suitable eddy viscosity coefficients, expressed in the φ, θ, p variables. Hence, for example,

$$L_v v = \mu_v \Delta v + \nu_v \frac{\partial}{\partial p} \left[\left(\frac{gp}{R\bar{T}} \right)^2 \frac{\partial v}{\partial p} \right] \quad [43]$$

with similar expressions for L_T and L_q . Note that F_T corresponds to the heating of the Sun, whereas F_v and F_q (which vanish in reality) are added here for mathematical generality. The change of variable gives, for $\partial^2 v / \partial z^2$, a term different from the coefficient of ν_v . The expression above is simplified for of this coefficient; the simplification is legitimate because ν_v is a very small coefficient (in particular, T has been replaced by \bar{T} (known) average value of the temperature).

Pseudogeometrical Domain

For physical and mathematical reasons, we do not allow the pressure to go to zero, and assume that $p \geq p_0$, with $p_0 > 0$ "small." Physically, in the very high atmosphere (p very small), the air is ionized and the equations above are not valid anymore. The pressure is then restricted to an interval $p_0 < p < p_1$, where p_1 is a value of the pressure smaller in average than the pressure on Earth, so that the isobar $p = p_1$ is slightly above the Earth and the isobar $p = p_0$ is an isobar high in the sky. We study the motion of the air between these two isobars.

For the whole atmosphere, the boundary of this domain

$$\mathcal{M} = \{(\varphi, \theta, p), p_0 < p < p_1\}$$

consists first of an upper part $\Gamma_u, p = p_0$; the lower part $p = p_1$ is divided into two parts Γ_i the part of $p = p_1$ at the interface with the ocean, and Γ_e the part of $p = p_1$ above the earth.

Boundary Conditions

Typically, the boundary conditions are as follows:

On the top of the atmosphere $\Gamma_u (p = p_0)$

$$\frac{\partial v}{\partial p} = 0, \quad \omega = 0, \quad \frac{\partial T}{\partial p} = 0, \quad \frac{\partial q}{\partial p} = 0 \quad [44]$$

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See also: Boundary Control Method and Inverse Problems of Wave Propagation; Compressible Flows: Mathematical Theory; Fluid Mechanics: Numerical Methods; Turbulence Theories.

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Gerbes in Quantum Field Theory

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Definitions and an Example

A gerbe can be viewed as a next step in a ladder of geometric and topological objects on a manifold which starts from ordinary complex-valued functions and in the second step of sections of complex line bundles.

It is useful to recall the construction of complex line bundles and their connections. Let M be a smooth manifold and $\{U_\alpha\}$ an open cover of M which trivializes a line bundle L over M . Topologically, up to equivalence, the line bundle is completely determined by its Chern class, which is a cohomology class $[c] \in H^2(M, \mathbb{Z})$. On each open set U_α we may write $2\pi ic = dA_\alpha$, where A_α is a 1-form. On the overlaps $U_{\alpha\beta} = U_\alpha \cap U_\beta$ we can write

$$A_\alpha - A_\beta = f_{\alpha\beta}^{-1} df_{\alpha\beta} \quad [1]$$

at least when $U_{\alpha\beta}$ is contractible, where $f_{\alpha\beta}$ is a circle-valued complex function on the overlap. The data $\{c, A_\alpha, f_{\alpha\beta}\}$ define what is known as a (representative of a) Deligne cohomology class on the open cover $\{U_\alpha\}$. The 1-forms A_α are the local

potentials of the curvature form $2\pi ic$ and the $f_{\alpha\beta}$'s are the transition functions of the line bundle L . Each of these three different data defines separately the equivalence class of the line bundle but together they define the line bundle with a connection.

The essential thing here is that there is a bijection between the second integral cohomology of M and the set of equivalence classes of complex line bundles over M . It is natural to ask whether there is a geometric realization of integral third (or higher) cohomology. In fact, gerbes provide such a realization. Here, we shall restrict to a smooth differential geometric approach which by no means is the most general possible, but it is sufficient for most applications to quantum field theory. However, there are examples of gerbes over orbifolds that do not need to come from finite group action on a manifold, which are not covered by the following definition.

For the examples in this article, it is sufficient to adapt the following definition. A gerbe over a manifold M (without geometry) is simply a principal bundle $\pi: P \rightarrow M$ with fiber equal to $PU(H)$, the projective unitary group of a Hilbert space H . The Hilbert space may be either finite or infinite dimensional.

The quantum field theory applications discussed in this article are related to the chiral anomaly for

fermions in external fields. The link comes from the fact that the chiral symmetry breaking leads in the generic case to projective representations of the symmetry groups. For this reason, when modding out by the gauge or diffeomorphism symmetries, one is led to study bundles of projective Hilbert spaces. The anomaly is reflected as a nontrivial characteristic class of the projective bundle, known in mathematics literature as the Dixmier–Douady class.

In a suitable open cover, the bundle P has a family of local trivializations with transition functions $g_{\alpha\beta}: U_{\alpha\beta} \rightarrow PU(H)$, with the usual cocycle property

$$g_{\alpha\beta}g_{\beta\gamma}g_{\gamma\alpha} = 1 \quad [2]$$

on triple overlaps. Assuming that the overlaps are contractible, we can choose lifts $\hat{g}_{\alpha\beta}: U_{\alpha\beta} \rightarrow U(H)$, to the unitary group of the Hilbert space. However,

$$\hat{g}_{\alpha\beta}\hat{g}_{\beta\gamma}\hat{g}_{\gamma\alpha} = f_{\alpha\beta\gamma} \quad [3]$$

where the f 's are circle-valued functions on triple overlaps. They satisfy automatically the cocycle property

$$f_{\alpha\beta\gamma}f_{\alpha\beta\delta}^{-1}f_{\alpha\gamma\delta}f_{\beta\gamma\delta}^{-1} = 1 \quad [4]$$

on quadruple overlaps. There is an important difference between the finite- and infinite-dimensional cases. In the finite-dimensional case, the circle bundle $U(H) \rightarrow U(H)/S^1 = PU(H)$ reduces to a bundle with fiber $\mathbb{Z}/N\mathbb{Z} = \mathbb{Z}_N$, where $N = \dim H$. This follows from $U(N)/S^1 = SU(N)/\mathbb{Z}_N$ and the fact that $SU(N)$ is a subgroup of $U(N)$. For this reason one can choose the lifts $\hat{g}_{\alpha\beta}$ such that the functions $f_{\alpha\beta\gamma}$ take values in the finite subgroup $\mathbb{Z}_N \subset S^1$.

The functions $f_{\alpha\beta\gamma}$ define an element $a = \{a_{\alpha\beta\gamma\delta}\}$ in the Čech cohomology $H^3(\mathcal{U}, \mathbb{Z})$ by a choice of logarithms,

$$2\pi i a_{\alpha\beta\gamma\delta} = \log f_{\alpha\beta\gamma} - \log f_{\alpha\beta\delta} + \log f_{\alpha\gamma\delta} - \log f_{\beta\gamma\delta} \quad [5]$$

In the finite-dimensional case, the Čech cocycle is necessarily torsion, $Na = 0$, but not so if H is infinite dimensional. In the finite-dimensional case (by passing to a good cover and using the Čech – de Rham equivalence over real or complex numbers), the class is third de Rham cohomology constructed from the transition functions is necessarily zero. Thus, in general one has to work with Čech cohomology to preserve torsion information. One can prove:

Theorem *The construction above is a one-to-one map between the set of equivalence classes of $PU(H)$ bundles over M and elements of $H^3(M, \mathbb{Z})$.*

The characteristic class in $H^3(M, \mathbb{Z})$ of a $PU(H)$ bundle is called the *Dixmier–Douady class*.

First example

Let M be an oriented Riemannian manifold and FM its bundle of oriented orthonormal frames. The structure group of FM is the rotation group $SO(n)$ with $n = \dim M$. The spin bundle (when it exists) is a double covering $\text{Spin}(M)$ of FM , with structure group $\text{Spin}(n)$, a double cover of $SO(n)$. Even when the spin bundle does not exist there is always the bundle $\text{Cl}(M)$ of Clifford algebras over M . The fiber at $x \in M$ is the Clifford algebra defined by the metric g_x , that is, it is the complex 2^n -dimensional algebra generated by the tangent vectors $v \in T_x(M)$ with the defining relations

$$\gamma(u)\gamma(v) + \gamma(v)\gamma(u) = 2g_x(u, v)$$

The Clifford algebra has a faithful representation in $N = 2^{\lfloor n/2 \rfloor}$ dimensions ($\lfloor x \rfloor$ is the integral part of x) such that

$$\gamma(a \cdot u) = S(a)\gamma(u)S(a)^{-1}$$

where S is an unitary representation of $\text{Spin}(n)$ in \mathbb{C}^N . Since $\text{Spin}(n)$ is a double cover of $SO(n)$, the representation S may be viewed as a projective representation of $SO(n)$. Thus again, if the overlaps $U_{\alpha\beta}$ are contractible, we may choose a lift of the frame bundle transition functions $g_{\alpha\beta}$ to unitaries $\hat{g}_{\alpha\beta}$ in $H = \mathbb{C}^N$. In this case, the functions $f_{\alpha\beta\gamma}$ reduce to \mathbb{Z}_2 -valued functions, and the obstruction to the lifting problem, which is the same as the obstruction to the existence of spin structure, is an element of $H^2(M, \mathbb{Z}_2)$, known as the second Stiefel–Whitney class w_2 . The image of w_2 with respect to the Bockstein map (in this case, given by the formula [5]) gives a 2-torsion element in $H^3(M, \mathbb{Z})$, the Dixmier–Douady class.

Another way to think of a gerbe is the following (we shall see that this arises in a natural way in quantum field theory). There is a canonical complex line bundle L over $PU(H)$, the associated line bundle to the circle bundle $S^1 \rightarrow U(H) \rightarrow PU(H)$. Pulling back L by the local transition functions $g_{\alpha\beta} \rightarrow PU(H)$, we obtain a family of line bundles $L_{\alpha\beta}$ over the open sets $U_{\alpha\beta}$. By the cocycle property [2] we have natural isomorphisms

$$L_{\alpha\beta} \otimes L_{\beta\gamma} = L_{\alpha\gamma} \quad [6]$$

We can take this as a definition of a gerbe over M : a collection of line bundles over intersections of open sets in an open cover of M , satisfying the cocycle condition [6]. By [6] we have a trivialization

$$L_{\alpha\beta} \otimes L_{\beta\gamma} \otimes L_{\gamma\alpha} = f_{\alpha\beta\gamma} \cdot 1 \quad [7]$$

where the f 's are circle-valued functions on the triple overlaps. By the theorem above, we conclude

that indeed the data in [6] define (an equivalence class of) a principal $PU(H)$ bundle.

If $L_{\alpha\beta}$ and $L'_{\alpha\beta}$ are two systems of local line bundles over the same cover, then the gerbes are equivalent if there is a system of line bundles L_α over open sets U_α such that

$$L'_{\alpha\beta} = L_{\alpha\beta} \otimes L_\alpha^* \otimes L_\beta \quad [8]$$

on each $U_{\alpha\beta}$.

A gerbe may come equipped with geometry, encoded in a Deligne cohomology class with respect to a given open covering of M . The Deligne class is given by functions $f_{\alpha\beta\gamma}$, 1-forms $A_{\alpha\beta}$, 2-forms F_α , and a global 3-form (the Dixmier–Douady class of the gerbe) Ω , subject to the conditions

$$\begin{aligned} dF_\alpha &= 2\pi i \Omega \\ F_\alpha - F_\beta &= dA_{\alpha\beta} \\ A_{\alpha\beta} - A_{\alpha\gamma} + A_{\beta\gamma} &= f_{\alpha\beta\gamma}^{-1} df_{\alpha\beta\gamma} \end{aligned} \quad [9]$$

Gerbes from Canonical Quantization

Let D_x be a family of self-adjoint Fredholm operators in a complex Hilbert space H parametrized by $x \in M$. This situation arises in quantum field theory, for example, when M is some space of external fields, coupled to Dirac operator D on a compact manifold. The space M might consist of gauge potentials (modulo gauge transformations) or M might be the moduli space of Riemann metrics. In these examples, the essential spectrum of D_x is both positive and negative and the family D_x defines an element of $K^1(M)$. In fact, one of the definitions of $K^1(M)$ is that its elements are homotopy classes of maps from M to the space \mathcal{F}_* of self-adjoint Fredholm operators with both positive and negative essential spectrum. In physics applications, one deals most often with unbounded Hamiltonians, and the operator norm topology must be replaced by something else; popular choices are the Riesz topology defined by the map $F \mapsto F/(|F| + 1)$ to bounded operators or the gap topology defined by graph metric.

The space \mathcal{F}_* is homotopy equivalent to the group $G = U_1(H)$ of unitary operators g in H such that $g - 1$ is a trace-class operator. This space is a classifying space for principal U_{res} bundles, where U_{res} is the group of unitary operators g in a polarized complex Hilbert space $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ such that the off-diagonal blocks of g are Hilbert–Schmidt operators. This is related to Bott periodicity. There is a natural principal bundle P over $G = U_1(H)$ with fiber equal to the group ΩG of based loops in G . The total

space P consists of smooth paths $f(t)$ in G starting from the neutral element such that $f^{-1}df$ is smooth and periodic. The projection $P \rightarrow G$ is the evaluation at the end point $f(1)$. The fiber is clearly ΩG . By Bott periodicity, the homotopy groups of ΩG are shifted from those of G by one dimension, that is,

$$\pi_n \Omega G = \pi_{n+1} G$$

The latter are zero in even dimensions and equal to \mathbb{Z} in odd dimensions. On the other hand, it is known that the even homotopy groups of $U_{\text{res}}(\mathcal{H})$ are equal to \mathbb{Z} and the odd ones vanish. In fact, with a little more effort, one can show that the embedding of ΩG to $U_{\text{res}}(\mathcal{H})$ is a homotopy equivalence, when $\mathcal{H} = L^2(S^1, H)$, the polarization being the splitting to non-negative and negative Fourier modes and the action of ΩG is the pointwise multiplication on H -valued functions on the circle S^1 .

Since P is contractible, it is indeed the classifying bundle for U_{res} bundles. Thus, we conclude that “ $K^1(M)$ = the set of homotopy classes of maps $M \rightarrow G$ = the set of equivalence classes of U_{res} bundles over M .” The relevance of this fact in quantum field theory follows from the properties of representations of the algebra of canonical anti-commutation relations (CAR). For any complex Hilbert space H , this algebra is the algebra generated by elements $a(v)$ and $a^*(v)$, with $v \in H$, subject to the relations

$$a^*(u)a(v) + a(v)a^*(u) = 2 \langle v, u \rangle$$

where the Hilbert space inner product on the right-hand side is antilinear in the first argument, and all other anticommutators vanish. In addition, $a^*(u)$ is linear and $a(v)$ antilinear in its argument.

An irreducible Dirac representation of the CAR algebra is given by a polarization $H = H_+ \oplus H_-$. The representation is characterized by the existence of a vacuum vector ψ in the fermionic Fock space \mathcal{F} such that

$$a^*(u)\psi = 0 = a(v)\psi \quad \text{for } u \in H_-, v \in H_+ \quad [10]$$

A theorem of D Shale and W F Stinespring says that two Dirac representations defined by a pair of polarizations H_+, H'_+ are equivalent if and only if there is $g \in U_{\text{res}}(H_+ \oplus H_-)$ such that $H'_+ = g \cdot H_+$. In addition, in order that a unitary transformation g is implementable in the Fock space, that is, there is a unitary operator \hat{g} in \mathcal{F} such that

$$\hat{g}a^*(v)\hat{g}^{-1} = a^*(gv), \quad \forall v \in H \quad [11]$$

and similarly for the $a(v)$'s, one must have $g \in U_{\text{res}}$ with respect to the polarization defining the vacuum vector. This condition is both necessary and sufficient.

The polarization of the one-particle Hilbert space comes normally from a spectral projection onto the positive-energy subspace of a Hamilton operator. In the background field problems one studies families of Hamilton operators D_x and then one would like to construct a family of fermionic Fock spaces parametrized by $x \in M$. If none of the Hamilton operators has zero modes, this is unproblematic. However, the presence of zero modes makes it impossible to define the positive-energy subspace $H_+(x)$ as a continuous function of x . One way out of this is to weaken the condition for the polarization: each $x \in M$ defines a Grassmann manifold $\text{Gr}_{\text{res}}(x)$ consisting of all subspaces $W \subset H$ such that the projections onto W and $H_+(x)$ differ by Hilbert-Schmidt operators. The definition of $\text{Gr}_{\text{res}}(x)$ is stable with respect to finite-rank perturbations of $D_x/|D_x|$. For example, when D_x is a Dirac operator on a compact manifold then $(D_x - \lambda)/|D_x - \lambda|$ defines the same Grassmannian for all real numbers λ because in each finite interval there are only a finite number of eigenvalues (with multiplicities) of D_x . From this follows that the Grassmannians form a locally trivial fiber bundle Gr over families of Dirac operators.

If the bundle Gr has a global section $x \mapsto W_x$ then we can define a bundle of Fock space representations for the CAR algebra over the parameter space M . However, there are important situations when no global sections exist. It is easier to explain the potential obstruction in terms of a principal U_{res} bundle P such that Gr is an associated bundle to P .

The fiber of P at $x \in M$ is the set of all unitaries g in H such that $g \cdot H_+ \in \text{Gr}_x$ where $H = H_+ \oplus H_-$ is a fixed reference polarization. Then we have

$$\text{Gr} = P \times_{U_{\text{res}}} \text{Gr}_{\text{res}},$$

where the right action of $U_{\text{res}} = U_{\text{res}}(H_+ \oplus H_-)$ in the fibers of P is the right multiplication on unitary operators and the left action on Gr_{res} comes from the observation that $\text{Gr}_{\text{res}} = U_{\text{res}}/(U_+ \times U_-)$, where U_{\pm} are the diagonal block matrices in U_{res} . By a result of N. Kuiper, the subgroup $U_- \times U_-$ is contractible and so Gr has a global section if and only if P is trivial.

Thus, when P is trivial we can define the family of Dirac representations of the CAR algebra parametrized by M such that in each of the Fock spaces we have a Dirac vacuum which, in a precise sense, is close to the vacuum defined by the energy polarization. However, the triviality of P is not a necessary condition. Actually, what is needed is that P has a prolongation to a bundle \hat{P} with fiber \hat{U}_{res} . The group \hat{U}_{res} is a central extension of U_{res} by the group S^1 .

The Lie algebra $\hat{\mathfrak{u}}_{\text{res}}$ is as a vector space the direct sum $\mathfrak{u}_{\text{res}} \oplus i\mathbb{R}$, with commutators

$$[X + \lambda, Y + \mu] = [X, Y] + c(X, Y) \quad [12]$$

where c is the Lie algebra cocycle

$$c(X, Y) = \frac{1}{4} \text{tr } \epsilon[\epsilon, X][\epsilon, Y] \quad [13]$$

Here ϵ is the grading operator with eigenvalues ± 1 on H_{\pm} . The trace exists since the off diagonal blocks of X, Y are Hilbert-Schmidt.

The group \hat{U}_{res} is a circle bundle over U_{res} . The Chern class of the associated complex line bundle is the generator of $H^2(U_{\text{res}}, \mathbb{Z})$ and is given explicitly at the identity element as the antisymmetric bilinear form $c/2\pi i$ and at other points on the group manifold through left-translation of $c/2\pi i$. If P is trivial, then it has an obvious prolongation to the trivial bundle $M \times \hat{U}_{\text{res}}$. In any case, if the prolongation exists we can define the bundle of Fock spaces carrying CAR representations as the associated bundle

$$\mathcal{F} = \hat{P} \times_{\hat{U}_{\text{res}}} \mathcal{F}_0$$

where \mathcal{F}_0 is the fixed Fock space defined by the same polarization $H = H_+ \oplus H_-$ used to define U_{res} . By the Shale-Stinespring theorem, any $g \in U_{\text{res}}$ has an implementation \hat{g} in \mathcal{F}_0 , but \hat{g} is only defined up to phase, thus the central S^1 extension.

The action of the CAR algebra in the fibers is given as follows. For $x \in M$ choose any $\hat{g} \in \hat{P}_x$. Define

$$a^*(v) \cdot (\hat{g}, \psi) = (\hat{g}, a^*(g^{-1}v)\psi)$$

where $\psi \in \mathcal{F}_0$ and $v \in H$; similarly for the operators $a(v)$. It is easy to check that this definition passes to the equivalence classes in \mathcal{F} . Note that the representations in different fibers are in general inequivalent because the transformation g is not implementable in the Fock space \mathcal{F}_0 .

The potential obstruction to the existence of the prolongation of P is again a 3-cohomology class on the base. Choose a good cover of M . On the intersections $U_{\alpha\beta}$ of the open cover the transition functions $g_{\alpha\beta}$ of P can be prolonged to functions $\hat{g}_{\alpha\beta}: U_{\alpha\beta} \rightarrow \hat{U}_{\text{res}}$. We have

$$\hat{g}_{\alpha\beta} \hat{g}_{\beta\gamma} \hat{g}_{\gamma\alpha} = f_{\alpha\beta\gamma} \cdot 1 \quad [14]$$

for functions $f_{\alpha\beta\gamma}: U_{\alpha\beta\gamma} \rightarrow S^1$, which by construction satisfy the cocycle property [4]. Since the cocycle is defined on a good cover, it defines an integral Čech cohomology class $\omega \in H^3(M, \mathbb{Z})$.

Let us return to the universal U_{res} bundle P over $G = U_1(H)$. In this case the prolongation obstruction can be computed relatively easily. It turns out that

the 3-cohomology class is represented by the de Rham class which is the generator of $H^3(G, \mathbb{Z})$. Explicitly,

$$\omega = \frac{1}{24\pi^2} \text{tr} (g^{-1} dg)^3 \quad [15]$$

Any principal U_{res} bundle over M comes from a pullback of P with respect to a map $f: M \rightarrow G$, so the Dixmier–Douady class in the general case is the pullback $f^*\omega$.

The line bundle construction of the gerbe over the parameter space M for Dirac operators is given by the observation that the spectral subspaces $E_{\lambda\lambda'}(x)$ of D_x , corresponding to the open interval $[\lambda, \lambda']$ in the real line, form finite-rank vector bundles over open sets $U_{\lambda\lambda'} = U_\lambda \cap U_{\lambda'}$. Here U_λ is the set of points $x \in M$ such that λ does not belong to the spectrum of D_x . Then we can define, as top exterior power,

$$L_{\lambda\lambda'} = \bigwedge^{\text{top}} (E_{\lambda\lambda'})$$

as the complex vector bundle over $U_{\lambda\lambda'}$. It follows immediately from the definition that the cocycle property [6] is satisfied.

Example 1 (Fermions on an interval). Let K be a compact group and ρ its unitary representation in a finite-dimensional vector space V . Let H be the Hilbert space of square-integrable V -valued functions on the interval $[0, 2\pi]$ of the real axis. For each $g \in K$ let $\text{Dom}_g \subset H$ be the dense subspace of smooth functions ψ with the boundary condition $\psi(2\pi) = \rho(g)\psi(0)$. Denote by D_g the operator $-\text{id}/dx$ on this domain. The spectrum of D_g is a function of the eigenvalues λ_k of $\rho(g)$, consisting of real numbers $n + \log(\lambda_k)/2\pi i$ with $n \in \mathbb{Z}$. For this reason the splitting of the one-particle space H to positive and negative modes of the operator D_g is in general not continuous as function of the parameter g . This leads to the problems described above. However, the principal U_{res} bundle can be explicitly constructed. It is the pullback of the universal bundle P with respect to the map $f: K \rightarrow G$ defined by the embedding $\rho(K) \subset G$ as $N \times N$ block matrices, $N = \dim V$. Thus, the Dixmier–Douady class in this example is

$$\omega = \frac{1}{24\pi^2} \text{tr} (\rho(g)^{-1} d\rho(g))^3 \quad [16]$$

Example 2 (Fermions on a circle). Let $H = L^2(S^1, V)$ and $D_A = -i(d/dx + A)$ where A is a smooth vector potential on the circle taking values in the Lie algebra \mathfrak{k} of K . In this case, the domain is fixed,

consisting of smooth V -valued functions on the circle. The \mathfrak{k} -valued function A is represented as a multiplication operator through the representation ρ of K . The parameter space \mathcal{A} of smooth vector potentials is flat; thus, there cannot be any obstruction to the prolongation problem. However, in quantum field theory, one wants to pass to the moduli space \mathcal{A}/\mathcal{G} of gauge potentials. Here \mathcal{G} is the group of smooth based gauge transformations, that is, $\mathcal{G} = \Omega K$. Now the moduli space is the group of holonomies around the circle, $\mathcal{A}/\mathcal{G} = K$. Thus, we are in a similar situation as in Example 1. In fact, these examples are really two different realizations of the same family of self-adjoint Fredholm operators. The operator D_A with $k = \text{holonomy}(A)$ has exactly the same spectrum as D_k in Example 1. For this reason, the Dixmier–Douady class on K is the same as before.

The case of Dirac operators on the circle is simple because all the energy polarizations for different vector potentials are elements in a single Hilbert–Schmidt Grassmannian $\text{Gr}(H_+ \oplus H_-)$, where we can take as the reference polarization the splitting to positive and negative Fourier modes. Using this polarization, the bundle of fermionic Fock spaces over \mathcal{A} can be trivialized as $\mathcal{F} = \mathcal{A} \times \mathcal{F}_0$. However, the action of the gauge group \mathcal{G} on \mathcal{F} acquires a central extension $\hat{\mathcal{G}} \subset \hat{LK}$, where LK is the free loop group of K . The Lie algebra cocycle determining the central extension is

$$c(X, Y) = \frac{1}{2\pi i} \int_{S^1} \text{tr}_\rho X dY \quad [17]$$

where tr_ρ is the trace in the representation ρ of K . Because of the central extension, the quotient $\mathcal{F}/\hat{\mathcal{G}}$ defines only a projective vector bundle over \mathcal{A}/\mathcal{G} , the Dixmier–Douady class being given by [16].

In the Example 1 (and Example 2) above, the complex line bundles can be constructed quite explicitly. Let us study the case $K = \text{SU}(n)$. Define $U_\lambda \subset K$ as the set of matrices g such that λ is not an eigenvalue of g . Select n different points λ_j on the unit circle such that their product is not equal to 1. We assume that the points are ordered counter-clockwise on the circle. Then the sets $U_j = U_{\lambda_j}$ form an open cover of $\text{SU}(n)$. On each U_j we can choose a continuous branch of the logarithmic function $\log: U_j \rightarrow \mathfrak{su}(n)$. The spectrum of the Dirac operator D_g with the holonomy g consists of the infinite set of numbers $\mathbb{Z} + \text{Spec}(-i \log(g))$. In particular, the numbers $\mathbb{Z} - i \log \lambda_j$ do not belong to the spectrum of D_g . Choosing $\mu_k = -i \log \lambda_k$ as an increasing sequence in the interval $[0, 2\pi]$, we can as well define $U_j = \{x \in M | \mu_j \notin \text{Spec}(D_x)\}$. In any case, the

top exterior power of the spectral subspace $E_{\mu_j, \mu_k}(x)$ is given by zero Fourier modes consisting of the spectral subspace of the holonomy g in the segment $[\lambda_j, \lambda_k]$ of the unit circle.

Index Theory and Gerbes

Gauge and gravitational anomalies in quantum field theory can be computed by Atiyah–Singer index theory. The basic setup is as follows. On a compact even-dimensional spin manifold S (without boundary) the Dirac operators coupled to vector potentials and metrics form a family of Fredholm operators. The parameter space is the set \mathcal{A} of smooth vector potentials (gauge connections) in a vector bundle over S and the set of smooth Riemann metrics on S . The family of Dirac operators is covariant with respect to gauge transformations and diffeomorphisms of S ; thus, we may view the Dirac operators parametrized by the moduli space \mathcal{A}/\mathcal{G} of gauge connections and the moduli space $\mathcal{M}/\text{Diff}_0(S)$ of Riemann metrics. Again, in order that the moduli spaces are smooth manifolds, one has to restrict to the based gauge transformations, that is, those which are equal to the neutral element in a fixed base point in each connected component of S . Similarly, the Jacobian of a diffeomorphism is required to be equal to the identity matrix at the base points. Passing to the quotient modulo gauge transformations and diffeomorphisms, we obtain a vector bundle over the space

$$S \times \mathcal{A}/\mathcal{G} \times \mathcal{M}/\text{Diff}_0(S) \quad [18]$$

Actually, we could as well consider a generalization in which the base space is a fibering over the moduli space with model fiber equal to S , but for simplicity we stick to [18].

According to the Atiyah–Singer index formula for families, the K-theory class of the family of Dirac operators acting on the smooth sections of the tensor product of the spin bundle and the vector bundle V over [18] is given through the differential forms

$$\hat{A}(R) \wedge \text{ch}(V)$$

where $\hat{A}(R)$ is the A-roof genus, a function of the Riemann curvature tensor R associated with the Riemann metric,

$$\hat{A}(R) = \det^{1/2} \left(\frac{R/4\pi i}{\sinh(R/4\pi i)} \right)$$

and $\text{ch}(V)$ is the Chern character

$$\text{ch}(V) = \text{tr} e^{F/2\pi i}$$

where F is the curvature tensor of a gauge connection. Here both R and F are forms on the infinite-dimensional base space [18]. After integrating over the fiber S ,

$$\text{Ind} = \int_S \hat{A}(R) \wedge \text{ch}(V) \quad [19]$$

we obtain a family of differential forms ϕ_{2k} , one in each even dimension, on the moduli space.

The (cohomology classes of) forms ϕ_{2k} contain important topological information for the quantized Yang–Mills theory and for quantum gravity. The form ϕ_2 describes potential chiral anomalies. The chiral anomaly is a manifestation of gauge or reparametrization symmetry breaking. If the class $[\phi_2]$ is nonzero, the quantum effective action cannot be viewed as a function on the moduli space. Instead, it becomes a section of a complex line bundle DET over the moduli space.

Since the Dirac operators are Fredholm (on compact manifolds), at a given point in the moduli space we can define the complex line

$$\text{DET}_x = \bigwedge^{\text{top}} (\ker D_x^+) \otimes \bigwedge^{\text{top}} (\text{coker } D_x^+) \quad [20]$$

for the chiral Dirac operators D_x^+ . In the even-dimensional case, the spin bundle is \mathbb{Z}_2 graded such that the grading operator Γ anticommutes with D_x . Then $D_x^+ = P_- D_x P_+$, where $P_{\pm} = (1/2)(1 \pm \Gamma)$ are the chiral projections. \bigwedge^{top} means the operation on finite-dimensional vector spaces W taking the exterior power of W to $\dim W$.

When the dimensions of the kernel and cokernel of D_x are constant, eqn [20] defines a smooth complex line bundle over the moduli space. In the case of varying dimensions, a little extra work is needed to define the smooth structure.

The form ϕ_2 is the Chern class of DET. So if DET is nontrivial, gauge covariant quantization of the family of Dirac operators is not possible.

One can also give a geometric and topological meaning to the chiral symmetry breaking in Hamiltonian quantization, and this leads us back to gerbes on the moduli space. Here we have to use an odd version of the index formula [19]. Assuming that the physical spacetime is even dimensional, at a fixed time the space is an odd-dimensional manifold S . We still assume that S is compact. In this case, the integration in [19] is over odd-dimensional fibers and, therefore, the formula produces a sequence of odd forms on the moduli space.

The first of the odd forms ϕ_1 gives the spectral flow of a one-parameter family of operators $D_{x(s)}$. Its integral along the path $x(t)$, after a correction by the difference of the eta invariant at the end points

of the path, in the moduli space, gives twice the difference of positive eigenvalues crossing over to the negative side of the spectrum minus the flow of eigenvalues in the opposite direction. The second term ϕ_3 is the Dixmier–Douady class of the projective bundle of Fock spaces over the moduli space. In Examples 1 and 2, the index theory calculation gives exactly the form [16] on K .

Example Consider Dirac operators on the three-dimensional sphere S^3 coupled to vector potentials. Any vector bundle on S^3 is trivial, so let $V = S^3 \times \mathbb{C}^N$. Take $SU(N)$ as the gauge group and let \mathcal{A} be the space of 1-forms on S^3 taking values in the Lie algebra $\mathfrak{su}(N)$ of $SU(N)$. Fix a point x_s on S^3 , the “south pole,” and let \mathcal{G} be the group of gauge transformations based at x_s . That is, \mathcal{G} consists of smooth functions $g: S^3 \rightarrow SU(N)$ with $g(x_s) = 1$. In this case \mathcal{A}/\mathcal{G} can be identified as $\text{Map}(S^2, SU(N))$ times a contractible space. This is because any point x on the equator of S^3 determines a unique semicircle from the south pole to the north pole through x . The parallel transport along this path with respect to a vector potential $A \in \mathcal{A}$ defines an element $g'_A(x) \in SU(N)$, using the fixed trivialization of V . Set $g_A(x) = g'_A(x)g'_A(x_0)^{-1}$, where x_0 is a fixed point on the equator. The element $g_A(x)$ then depends only on the gauge equivalence class $[A] \in \mathcal{A}/\mathcal{G}$. It is not difficult to show that the map $A \mapsto g_A$ is a homotopy equivalence from the moduli space of gauge potentials to the group $\mathcal{G}_2 = \text{Map}_{x_0}(S^2, SU(N))$, based at x_0 . When $N > 2$, the cohomology $H^5(SU(N), \mathbb{Z}) = \mathbb{Z}$ transgresses to the cohomology $H^3(\mathcal{G}_2, \mathbb{Z}) = \mathbb{Z}$. In particular, the generator

$$\omega_5 = \left(\frac{i}{2\pi}\right)^3 \frac{2}{5!} \text{tr}(g^{-1} dg)^5$$

of $H^5(SU(N), \mathbb{Z})$ gives the generator of $H^3(\mathcal{G}_2, \mathbb{Z})$ by contraction and integration,

$$\Omega = \int_{S^2} \omega_5$$

Gauge Group Extensions

The new feature for gerbes associated with Dirac operators in higher than one dimension is that the gauge group, acting on the bundle of Fock spaces parametrized by vector potentials, is represented through an abelian extension. On the Lie algebra level this means that the Lie algebra extension is not given by a scalar cocycle c as in the one-dimensional case but by a cocycle taking values in an abelian Lie algebra. In the case of Dirac operators coupled to vector potentials, the abelian Lie algebra consists of

a certain class of complex functions on \mathcal{A} . The extension is then defined by the commutators

$$[(X, \alpha), (Y, \beta)] = ([X, Y], \mathcal{L}_X \beta - \mathcal{L}_Y \alpha + c(X, Y)) \quad [21]$$

where α, β are functions on \mathcal{A} and $\mathcal{L}_X \beta$ denotes the Lie derivative of β in the direction of the infinitesimal gauge transformation X . The 2-cocycle property of c is expressed as

$$c([X, Y], Z) + \mathcal{L}_X c(Y, Z) + \text{cyclic permutations of } X, Y, Z = 0$$

In the case of Dirac operators on a 3-manifold S the form c is the Mickelsson–Faddeev cocycle

$$c(X, Y) = \frac{i}{12\pi^2} \int_S \text{tr}_\rho A \wedge (dX \wedge dY - dY \wedge dX) \quad [22]$$

The corresponding gauge group extension is an extension of $\text{Map}(S, G)$ by the normal subgroup $\text{Map}(\mathcal{A}, S^1)$. As a topological space, the extension is the product

$$\text{Map}(\mathcal{A}, S^1) \times_{S^1} P$$

where P is a principal S^1 bundle over $\text{Map}(S, G)$.

The Chern class c_1 of the bundle P is again computed by transgression from ω_5 ; this time

$$c_1 = \int_S \omega_5$$

In fact, we can think of the cocycle c as a 2-form on the space of flat vector potentials $A = g^{-1} dg$ with $g \in \text{Map}(S^3, G)$. Then one can show that the cohomology classes $[c]$ and $[c_1]$ are equal.

As we have seen, the central extension of a loop group is the key to understanding the quantum field theory gerbe. Here is a brief description of it starting from the 3-form [16] on a compact Lie group G . First define a central extension $\text{Map}(D, G) \times S^1$ of the group of smooth maps from the unit disk D to G , with pointwise multiplication. The group multiplication is given as

$$(g, \lambda) \cdot (g', \lambda') = (gg', \lambda\lambda' \cdot e^{2\pi i \gamma(g, g')})$$

where

$$\gamma(g, g') = \frac{1}{8\pi^2} \int_D \text{tr}_\rho g^{-1} dg \wedge dg' g'^{-1} \quad [23]$$

where the trace is computed in a fixed unitary representation ρ of G . This group contains as a normal subgroup the group N consisting of pairs $(g, e^{2\pi i C(g)})$ with

$$C(g) = \frac{1}{24\pi^2} \int_B \text{tr}_\rho (g^{-1} dg)^3 \quad [24]$$

Here $g(x) = 1$ on the boundary circle $S^1 = \partial D$, and thus can be viewed as a function $S^2 \rightarrow G$. The three-dimensional unit ball B has S^2 as a boundary and g is extended in an arbitrary way from the boundary to the ball B . The extension is possible since $\pi_2(G) = 0$ for any finite-dimensional Lie group. The value of $C(g)$ depends on the extension only modulo an integer and therefore $e^{2\pi i C(g)}$ is well defined.

The central extension is then defined as

$$\widehat{LG} = (\text{Map}(D, G) \times S^1)/N$$

One can show easily that the Lie algebra of \widehat{LG} is indeed given through the cocycle [17]. When $G = \text{SU}(n)$ in the defining representation, this central extension is the basic extension: The cohomology class is the generator of $H^2(LG, \mathbb{Z})$. In general, to obtain the basic extension one has to correct [23] and [24] by a normalization factor.

This construction generalizes to the higher loop groups $\text{Map}(S, G)$ for compact odd-dimensional manifolds S . For example, in the case of a 3-manifold, one starts from an extension of $\text{Map}(D, G)$, where D is a 4-manifold with boundary S . The extension is defined by a 2-cocycle γ , but now for given g, g' the cocycle γ is a real-valued function of a point $g_0 \in \text{Map}(S, G)$, which is a certain differential polynomial in the Maurer–Cartan 1-forms $g_0^{-1}dg_0, g^{-1}dg, g^{-1}dg$. The normal subgroup N is defined in a similar way; now $C(g)$ is the integral of the 5-form ω_5 over a 5-manifold B with boundary ∂B identified as D/\sim , the equivalence shrinking the boundary of D to one point. This gives the extension only over the connected component of identity in $\text{Map}(S, G)$, but it can be generalized to the whole group. For example, when $S = S^3$ and G is simple, the connected components are labeled by elements of the third homotopy group $\pi_3 G = \mathbb{Z}$.

In some cases, the de Rham cohomology class of the extension vanishes but the extension still contains interesting torsion information. In quantum field theory this comes from Hamiltonian

formulation of global anomalies. A typical example of this phenomenon is the Witten $\text{SU}(2)$ anomaly in four spacetime dimensions. In the Hamiltonian formulation, we take S^3 as the physical space, the gauge group $G = \text{SU}(2)$. In this case, the second cohomology of $\text{Map}(S^3, G)$ becomes pure torsion, related to the fact that the 5-form ω_5 on $\text{SU}(2)$ vanishes for dimensional reasons. Here the homotopy group $\pi_4(G) = \mathbb{Z}_2$ leads the nontrivial fundamental group \mathbb{Z}_2 in each connected component of $\text{Map}(S^3, G)$. Using this fact, one can show that there is a nontrivial \mathbb{Z}_2 extension of the group $\text{Map}(S^3, G)$.

See also: Anomalies; Bosons and Fermions in External Fields; Characteristic Classes; Dirac Operator and Dirac Field; Index Theorems; K -Theory.

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Ginzburg–Landau Equation

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Introduction

In the Ginzburg–Landau theory of superconductivity, a complex order parameter Ψ characterizes a macroscopic/mesoscopic superconducting state in a bulk superconductor. The square of the magnitude $|\Psi|^2$ expresses the density of superconducting electrons and Ψ is regarded as a macroscopic wave function. With a magnetic vector potential \mathbf{A} and the order parameter Ψ , the Helmholtz free energy density in a superconducting material near the critical temperature is given by

$$F = F_n + \alpha |\Psi|^2 + \frac{\beta}{2} |\Psi|^4 + \frac{1}{2m_s} \left| \left(-i\hbar \nabla - \frac{e_s}{c} \mathbf{A} \right) \Psi \right|^2 + \frac{|\mathbf{H}|^2}{8\pi}$$

where F_n denotes the energy density of the normal state, c is the light speed, $\mathbf{H} = \text{curl } \mathbf{A}$, and m_s and e_s are mass and charge of a superconducting electron, respectively. The parameters α and β depend on temperature and are determined by the material. Moreover, below the critical temperature T_c , $\alpha = \alpha(T)$ and $\beta = \beta(T)$ take negative and positive values, respectively. In the presence of an applied magnetic field \mathbf{H}_{ap} , we have to consider the Gibbs free energy density, $G = F - \mathbf{H} \cdot \mathbf{H}_{\text{ap}}/4\pi$.

Introduce the following physical parameters:

$$\begin{aligned} \Psi_0 &= \sqrt{-\alpha/\beta}, & H_c &= \sqrt{4\pi\alpha^2/\beta} \\ \lambda &= \sqrt{-\beta m_s c^2 / 4\pi\alpha e_s^2}, & \xi &= \sqrt{-\hbar^2 / 2m_s \alpha} \\ \kappa &= \lambda/\xi \end{aligned} \quad [1]$$

The value Ψ_0^2 implies the equilibrium density and H_c is the thermodynamic critical field, which is obtained by equating $G = F_n - |\mathbf{H}_{\text{ap}}|^2/8\pi$ (for the normal state $\Psi = 0$, $\mathbf{H} = \mathbf{H}_{\text{ap}}$) with $G = F_n - \alpha^2/2\beta$ (for the perfect superconductivity $|\Psi|^2 = \Psi_0^2$, $\mathbf{A} = 0$). The parameters λ and ξ stand for penetration depth and coherence length, respectively. The ratio κ of these characteristic lengths is called the Ginzburg–Landau parameter, which determines the type of superconducting material: type I for $\kappa < 1/\sqrt{2}$ and type II for $\kappa > 1/\sqrt{2}$.

We use the nondimensional variables x', Ψ', \mathbf{A}' , \mathbf{H}_{ap}' , and \tilde{G} :

$$\begin{aligned} x &= \lambda x', & \Psi &= \Psi_0 \Psi' \\ \mathbf{A} &= \sqrt{2} H_c \xi \mathbf{A}' \quad (\mathbf{H}' = \text{curl}' \mathbf{A}'), \\ \mathbf{H}_{\text{ap}} &= \sqrt{2} H_c \mathbf{H}_{\text{ap}}' / \kappa \\ F &= F_n + (\tilde{G}/\kappa^2 - 1/2 \\ &\quad + 2\mathbf{H}' \cdot \mathbf{H}_{\text{ap}}' / \kappa^2 - |\mathbf{H}_{\text{ap}}'|^2 / \kappa^2) H_c^2 / 4\pi \end{aligned} \quad [2]$$

Dropping the primes after the change of variables and integrating \tilde{G} over a domain $\Omega \subset \mathbb{R}^n (n=2, 3)$, which is occupied by a superconducting sample, yields a functional of Ψ and \mathbf{A} , called the Ginzburg–Landau energy in a nondimensional form,

$$E(\Psi, \mathbf{A}) = \int_{\Omega} \left\{ |(\nabla - i\mathbf{A})\Psi|^2 + \frac{\kappa^2}{2} (1 - |\Psi|^2)^2 + |\text{curl } \mathbf{A} - \mathbf{H}_{\text{ap}}|^2 \right\} dx \quad [3]$$

The Ginzburg–Landau equations are the Euler–Lagrange equations of this energy, which are given by

$$(\nabla - i\mathbf{A})^2 \Psi = \kappa^2 (|\Psi|^2 - 1) \quad \text{in } \Omega \quad [4]$$

$$\text{curl}^2 \mathbf{A} = \mathbf{J} + \text{curl } \mathbf{H}_{\text{ap}} \quad \text{in } \Omega \quad [5]$$

where

$$\mathbf{J} := \frac{1}{2i} (\Psi^* \nabla \Psi - \Psi \nabla \Psi^*) - |\Psi|^2 \mathbf{A} \quad [6]$$

Ψ^* stands for the complex conjugate of Ψ . In a two-dimensional domain Ω , the differential operator “curl” acts on $\mathbf{A} = (A_1, A_2) : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ such that

$$\begin{aligned} \text{curl } \mathbf{A} &= \partial_{x_1} A_2 - \partial_{x_2} A_1 \\ \text{curl } \mathbf{H} &= (\partial_{x_2} H, -\partial_{x_1} H) \\ \mathbf{H} &:= \text{curl } \mathbf{A} \end{aligned}$$

and \mathbf{H}_{ap} is replaced by a scalar-valued function. Note that \mathbf{J} represents a supercurrent in the material. Every critical point of the energy is obtained by solving the Ginzburg–Landau equations with appropriate boundary conditions and, thus, a physical state in the superconducting sample is realized by a solution of the equations. A minimizer of [3] is a solution of [4]–[5] that minimizes the energy [3] in an appropriate function space, whereas a local minimizer is a solution minimizing the energy locally in the space. A solution is called a stable solution if it is a local minimizer of the energy. A physically stable phenomenon could be realized by a minimizer or at least a local minimizer.

The Ginzburg–Landau energy and the equations are gauge invariant under the transformation

$$(\Psi, \mathbb{A}) \mapsto (\Psi e^{i\chi}, \mathbb{A} + \nabla \chi) \quad [7]$$

for a smooth scalar function $\chi(x)$. Therefore, we can identify two solutions which have the correspondence through the transformation [7]. The following London (Coulomb) gauge is often chosen:

$$\operatorname{div} \mathbb{A} = 0 \quad \text{in } \Omega \quad [8]$$

(with a boundary condition if necessary).

Let (Ψ, \mathbb{A}) be a smooth solution of [4]–[5]. In a region for $|\Psi(x)| > 0$, the expression $\Psi = w(x) \exp(i\theta(x))$ ($w = |\Psi(x)|$) leads to

$$\nabla^2 w = |\nabla \theta - \mathbb{A}|^2 w + \kappa^2(w^2 - 1)w \quad [9]$$

$$\operatorname{div}(w^2(\nabla \theta - \mathbb{A})) = 0 \quad [10]$$

$$\operatorname{curl}^2 \mathbb{A} = \mathbb{J} = w^2(\nabla \theta - \mathbb{A}) \quad [11]$$

where the gauge [8] is fixed and $\operatorname{curl} \mathbb{H}_{\text{ap}} = 0$ is assumed. Let S be a surface in Ω bounded by a closed curve ∂S . Suppose $w(x) > 0$ on ∂S . Then from [11],

$$\begin{aligned} \Phi &:= \int_{\partial S} (\mathbb{J}/w^2 + \mathbb{A}) \cdot ds \\ &= \int_{\partial S} \frac{1}{w^2} \mathbb{J} \cdot ds + \int_S \operatorname{curl} \mathbb{A} \cdot dS \\ &= \int_{\partial S} \nabla \theta \cdot ds = 2d\pi \end{aligned} \quad [12]$$

where d is an integer; in fact, $d = \deg(\Psi, \partial S)$ is the winding number of $\Psi(\partial S)$ in the complex plane. Thus, the identity [12] relates the magnetic field to a topological degree of the order parameter. The quantity Φ , multiplied by an appropriate constant, is called the fluxoid. A connected component of vanishing points of Ψ generally has codimension 2 in the domain, and it is called a vortex.

From the expression [9], the asymptotic behavior $w \rightarrow 1$ as $\kappa \rightarrow \infty$ is expected under a suitable condition. Then, by [11], $\mathbb{H} = \operatorname{curl} \mathbb{A}$ enjoys the property $\operatorname{curl}^2 \mathbb{H} + \operatorname{curl} \mathbb{H} = 0$, which is known as the London equation. However, this is valid for $|\Psi| > 0$. Otherwise, a singularity appears around zeros of Ψ .

There are several characteristic phenomena observed in a bulk superconductor. Typical phenomena are: perfect conductivity (persistent current), perfect diamagnetism (Meissner effect), nucleation of superconductivity, and vortices (quantization of a penetrating magnetic field). These phenomena can be expressed by solutions of the Ginzburg–Landau equations in various settings.

Ginzburg–Landau Equations in \mathbb{R}^2

A standard model of the Ginzburg–Landau energy is considered in the whole space \mathbb{R}^2 . Let $\mathbb{A} = (A_1, A_2)$ and assume $\mathbb{H}_{\text{ap}} = 0$ in [3]. Consider then the energy functional

$$\begin{aligned} \mathcal{E}(\Psi, \mathbb{A}) &= \int_{\mathbb{R}^2} |D_A \Psi|^2 + |\operatorname{curl} \mathbb{A}|^2 \\ &\quad + \frac{\kappa^2}{2} (1 - |\Psi|^2)^2 dx \end{aligned} \quad [13]$$

where $D_A := \nabla - i\mathbb{A}$. Then the Ginzburg–Landau equations are

$$D_A^2 \Psi = \kappa^2(|\Psi|^2 - 1)\Psi \quad \text{in } \mathbb{R}^2 \quad [14]$$

$$\operatorname{curl}^2 \mathbb{A} = \operatorname{Im}(\Psi^* D_A \Psi) \quad \text{in } \mathbb{R}^2 \quad [15]$$

In the gauge theory, this model can be regarded as a two-dimensional abelian ($U(1)$) Higgs model. In that context, Ψ is a scalar (Higgs) field, \mathbb{A} is a connection on the $U(1)$ bundle $\mathbb{R}^2 \times U(1)$, and D_A is the covariant derivative.

Equations [14]–[15] are useful in observing quantization of the magnetic field, although it is an ideal model for superconductivity. By the natural condition that the right-hand side of [13] is finite, we may assume that $|D_A \Psi|, |\operatorname{curl} \mathbb{A}| \rightarrow 0$ and $|\Psi| \rightarrow 1$ as $|x| \rightarrow \infty$. From [12], the flux quantization follows:

$$\int_{\mathbb{R}^2} \operatorname{curl} \mathbb{A} dx = 2d\pi \quad [16]$$

If Ψ has a finite number of zeros $\{a_j\}_{j=1}^N$, [16] implies

$$\int_{\mathbb{R}^2} \operatorname{curl} \mathbb{A} dx = 2\pi \sum_{j=1}^N \deg(\Psi, \partial B(a_j, \rho))$$

for a small positive number ρ , where $B(a_j, \rho)$ stands for the disk with the center a_j and the radius ρ . A zero of Ψ represents a vortex, at which the magnetic field is quantized, and a supercurrent moves around the field.

To characterize the configuration analytically, we find a solution (Ψ, \mathbb{A}) expressed by the polar coordinate in the form

$$\Psi = f(r) \exp(id\theta), \quad \mathbb{A}(r) = \alpha(r)(-\sin \theta, \cos \theta)$$

Substituting these into [14]–[15], one obtains

$$\begin{aligned} \frac{1}{r}(rf')' - \left(\frac{d}{r} - \alpha\right)^2 f &= \kappa^2(f^2 - 1)f \\ \left(\frac{1}{r}(r\alpha)'\right)' &= f^2 \left(\alpha - \frac{d}{r}\right) \end{aligned}$$

($' = d/dr$) with the boundary conditions

$$f(0) = 0, \quad f(\infty) = 1, \quad \alpha(\infty) = 0$$

This system of the equations has a solution for $\kappa > 0$. In addition to these types of solutions, when $\kappa = 1/\sqrt{2}$, a special transformation reduces the system of [14]–[15] to a scalar nonlinear equation with a singular term. Then, it is proved that for an arbitrary $d \in \mathbb{Z}$, under the constraint of [16] there exists a minimizer of [13] with zeros of prescribed points $\{a_j\}_{j=1}^{|d|}$ (Jaffe and Taubes 1980).

Solutions for Persistent Current

A current flowing in a superconducting ring with no decay even in the absence of an applied magnetic field is called a persistent current. Assume that a superconducting sample Ω in \mathbb{R}^3 is surrounded by vacuum and adopt the energy functional as

$$\mathcal{E}(\Psi, \mathbb{A}) = \int_{\Omega} |D_A \Psi|^2 + \frac{\kappa^2}{2} (1 - |\Psi|^2)^2 dx + \int_{\mathbb{R}^3} |\text{curl } \mathbb{A}|^2 \quad [17]$$

Although the functional [17] is minimized by a trivial solution $(\Psi, \mathbb{A}) = (\exp(ic), 0)$ ($c \in \mathbb{R}$), which is the case for perfect diamagnetism, this is not the solution describing a persistent current since $\mathbb{J} = 0$ everywhere. We have to look for a nontrivial solution that locally minimizes the energy, that is, a local minimizer of [17]. To characterize a solution representing the persistent current, we define a mapping from Ω to $S^1 \subset \mathbb{C}$ by $x \in \Omega \rightarrow \Psi(x)/|\Psi(x)|$ for a solution (Ψ, \mathbb{A}) of the corresponding Ginzburg–Landau equations to [17]. Consider a domain having infinitely many homotopy classes in the space of continuous functions $C^0(\bar{\Omega}, S^1)$ (e.g., a solid torus). If (Ψ, \mathbb{A}) is a local minimizer and $\Psi/|\Psi|$ is not homotopic to a constant map of $C^0(\bar{\Omega}, S^1)$, then it is a solution describing a persistent current. The existence of such a solution has been established mathematically for large κ (Jimbo and Morita 1996, Rubinstein and Sternberg 1996).

Configuration of Solutions under an Applied Magnetic Field

In the presence of an applied magnetic field, according to the magnitude of the field, a sample exhibits the transition from the superconducting state to the normal state and vice versa. This transition can be considered mathematically as a bifurcation of solutions to the Ginzburg–Landau equations with a parameter measuring the magnitude of the applied magnetic field. In fact, let H_{ap} be an applied magnetic field perpendicular to the

horizontal plane and assume that it is constant along the vertical axis, that is, $H_{\text{ap}} = (0, 0, H_a)$. Then a rich bifurcation structure is suggested by numerical and analytical studies in the parameter space of (H_a, κ) . Mathematical developments for variational methods and nonlinear analysis reveal the configuration of the solutions and provide rigorous estimates for critical fields in a parameter regime for a two-dimensional model, predicted by physicists.

Throughout this section, we consider the Ginzburg–Landau model in an infinite cylinder $\Omega = D \times \mathbb{R}$ ($D \subset \mathbb{R}^2$) with a constant applied magnetic field $H_{\text{ap}} = H_a e_3 = (0, 0, H_a)$, $H_a > 0$. Assuming the uniformity along the vertical axis, we may write $\mathbb{A} = (A_1, A_2)$ and $H = \text{curl } \mathbb{A} = \partial_{x_1} A_2 - \partial_{x_2} A_1$ as in the previous section. Then the Ginzburg–Landau energy on D is

$$\mathcal{E}(\Psi, \mathbb{A}) = \int_D \left\{ |D_A \Psi|^2 + \frac{\kappa^2}{2} (1 - |\Psi|^2)^2 + |\text{curl } \mathbb{A} - H_a|^2 \right\} dx \quad [18]$$

With the London gauge

$$\text{div } \mathbb{A} = 0 \quad \text{in } D, \quad \mathbb{A} \cdot \mathbf{n} = 0 \quad \text{on } \partial D$$

the Ginzburg–Landau equations in the present setting are written as

$$D_A^2 \Psi = (|\Psi|^2 - 1)\Psi \quad \text{in } D \quad [19]$$

$$-\nabla^2 \mathbb{A} = \text{Im}(\Psi^* D_A \Psi) \quad \text{in } D \quad [20]$$

$$\mathbf{n} \cdot \nabla \Psi = 0 \quad \text{on } \partial D \quad [21]$$

$$\text{curl } \mathbb{A} = H_a \quad \text{on } \partial D \quad [22]$$

where \mathbf{n} denotes the outer unit normal.

Meissner Solutions

As seen in the case of no applied magnetic field, the trivial solution $(\Psi, \mathbb{A}) = (\exp(ic), 0)$ is a minimizer of [18]. This solution expresses no magnetic field in the sample. In a superconducting sample, the diamagnetism holds even in the presence of an applied magnetic field if the field is weak. Namely, the sample is shielded so that penetration of the field is only allowed near the surface of the sample. This phenomenon is called the Meissner effect. A solution expressing Meissner effect is called a Meissner solution. Mathematically, it is understood that as H_a increases, such a Meissner solution continues from the trivial solution. Then the solution preserves the configuration $0 < |\Psi(x)| < 1$. A study of the asymptotic behavior of the Meissner solution as κ tends to ∞ shows that the Meissner solution is a

minimizer up to $H_a = O(\log \kappa)$ for sufficiently large κ (Serfaty 1999).

Nucleation of Superconductivity

In an experiment, the Meissner state breaks down by a stronger applied magnetic field. Then the sample turns to be the normal state (in a type I conductor) or it allows a mixed state of superconductivity and normal state (in a type II conductor). In the former case, the critical magnitude of the field is denoted by H_c , which corresponds to the one of [1], while it is denoted by H_{c1} in the latter case. Moreover, the mixed state eventually breaks down to be normal state by further increasing the applied field up to another critical field H_{c2} . To characterize these two types mathematically, we consider a transition from the normal state to the superconducting state by reducing the magnitude of the field.

Let \mathbb{A}_{ap} satisfy $\text{curl } \mathbb{A}_{\text{ap}} = H_a (x \in D)$ and $\mathbb{A}_{\text{ap}} \cdot \mathbf{n} = 0 (x \in \partial D)$. Then eqns [19]–[22] have a trivial solution $(\Psi, \mathbb{A}) = (0, \mathbb{A}_{\text{ap}})$, which stands for the normal state. Consider the second variation of the energy functional [18] at this trivial solution

$$\frac{1}{2} \frac{d^2}{ds^2} E(s\psi, \mathbb{A}_{\text{ap}} + s\mathbb{B}) \Big|_{s=0} = \int_D |(\nabla - i\mathbb{A}_{\text{ap}})\psi|^2 - \kappa^2 |\psi|^2 + |\text{curl } \mathbb{B}|^2 dx$$

If the minimum of this second variation for nonzero (ψ, \mathbb{B}) is positive (or negative), then the trivial solution is stable (or unstable). The minimum gives the least eigenvalue of the linearized problem of [19]–[20] around the trivial solution. Seeking such a least eigenvalue μ is reduced to studying an eigenvalue problem of the Schrödinger operator $L[\psi] := -(\nabla - i\mathbb{A}_{\text{ap}})^2 \psi$.

If the domain D is the whole space \mathbb{R}^2 , it is proved that $\mu = H_a$. Back to the original variable of [2], we can define a critical field $H_{c2} = \sqrt{2}H_c\kappa$; $\kappa = 1/\sqrt{2}$ separates a class of superconductors into type I by $\kappa < 1/\sqrt{2}$ ($H_{c2} < H_c$) and type II by $\kappa > 1/\sqrt{2}$ ($H_{c2} > H_c$).

In the bounded domain D , however, the critical field at which superconductivity nucleates in the interior of a sample is larger than H_{c2} (it is denoted by H_{c3}), since the eigenvalue problem of L is considered in the domain with the Neumann boundary condition. A study of the least eigenvalue μ shows that the critical field has the asymptotics as

$$H_{c3}/\sqrt{2}H_c = \frac{\kappa}{\beta} + O(1), \quad \kappa \rightarrow \infty$$

where $0 < \beta < 1$. If the applied field is very close to H_{c3} and κ is sufficiently large, the amplitude of the eigenfunction associated with the least eigenvalue of

L (with the Neumann boundary condition) is very small except for a $1/\kappa$ neighborhood of the boundary. This implies that the nucleation of superconductivity takes place at the boundary. This phenomenon is called surface nucleation (Del Pino *et al.* 2000, Lu and Pan 1999).

Solutions of Vortices

In a type II superconductor, it is well known that there exists a mixed state of superconductivity and normal state in a parameter regime $H_{c1} < H_a < H_{c2}$. In the mixed state, the magnetic field penetrating in the sample is quantized such that it delivers a finite number of lines or curves in the sample. This configuration (called vortex) is characterized by zero sets of the order parameter of the Ginzburg–Landau equations. In a two-dimensional domain, isolating vanishing points of the order parameter are called vortices. Thus, it is quite an interesting problem how such a vortex configuration can be described mathematically by a minimizer of the energy functional. In the section “Ginzburg–Landau equations in \mathbb{R}^2 ,” a specific configuration for vortex solutions is stated under very special conditions, $\kappa = 1/\sqrt{2}$, on the whole space and no applied magnetic field. However, this result is not generalized in the present setting.

A standard approach to a solution with the vortex configuration is using a bifurcation analysis near the critical field H_{c2} (or H_{c3}) by expanding a solution and the difference $H_a - H_{c2}$ in a small parameter. Then the leading term is given by an eigenfunction of the least eigenvalue of the Schrödinger operator coming from the linearization. Under the doubly periodic conditions in the whole space \mathbb{R}^2 , the spatial pattern of vortices, called Abrikosov’s vortex lattice, is studied by a local bifurcation theory.

However, this kind of bifurcation analysis only works near the critical field and the trivial solution $(\Psi, \mathbb{A}) = (0, \mathbb{A}_{\text{ap}})$, which implies that only a small-amplitude solution can be found. To realize a sharp configuration of vortices, we need to consider a parameter regime far from the bifurcation point. As a matter of fact, mathematical and numerical studies for sufficiently large κ exhibit nice configurations of vortex solutions. In this case, in a neighborhood of each vortex, with radius $O(1/\kappa)$, a sharp layer arises, and there exists a solution with multivortices in an appropriate parameter region for H_a . In addition, as H_a increases (up to H_{c2}), the number of vortices also increases. This implies that the minimizer of the energy functional [18] admits a larger number of zeros for a higher magnitude of applied magnetic field. However, it is a puzzle since

a solution with a smaller number of vortices seems to have less energy. Thus, there is some balance mechanism between contributions of the vortices and the applied magnetic field to the total energy.

Mathematically, it is possible to estimate $\mathcal{E}(\Psi, \mathbb{A})$ for the vortex solution to [19]–[22] as follows: consider a family of square tiles K_j with side-length ρ which are periodically arranged over the whole space. Assume each square in the domain D has a single vortex. For an appropriate test function, the energy over K_j is estimated as $O(\log(\kappa\rho))$. Since the number of vortices in the domain is $O(|D|/\rho^2)$ ($|D|$: the measure of D), we obtain an upper bound $O(|D|/\rho^2 \log(\kappa\rho))$. This bound is less than $\mathcal{E}(0, \mathbb{A}_{\text{ap}}) = |D|\kappa^2/2$ for $H_a/\kappa^2 = o(1)$ and $\rho = 1/\sqrt{H_a}$. Although in a general case it is difficult to estimate the energy of the minimizer from below, the leading order can be precisely determined in some range of the interval (H_{c1}, H_{c2}) if κ is sufficiently large (Sandier and Serfaty 2000).

A Simplified Model

Since the Ginzburg–Landau equations [4]–[5] are coupled equations for Ψ and \mathbb{A} , we often encounter mathematical difficulty in realizing a solution with the configuration shown by a numerical experiment. To look at a specific configuration, we may use a simpler model equation. A typical simplification is to neglect the magnetic field, which leads to the equation for the order parameter ψ :

$$\nabla^2 \psi + \kappa^2(1 - |\psi|^2)\psi = 0 \quad \text{in } \Omega \quad [23]$$

This equation is also called the Ginzburg–Landau equation and it is the Euler–Lagrange equation of the energy

$$G(\psi) = \int_{\Omega} |\nabla \psi|^2 + \frac{\kappa^2}{2}(1 - |\psi|^2)^2 dx \quad [24]$$

in an appropriate function space. Under no constraint, a constant solution with $|\psi| = 1$ is a minimizer. If a domain is topologically nontrivial, eqn [23] also allows local minimizers of [24] for large κ as seen in the section “Solutions for Persistent Current.”

On the other hand, [23] in a simply connected domain $D \subset \mathbb{R}^2$ with a boundary condition $\psi = g(x)$ ($x \in \partial D$) is used for a study of a vortex solution for large κ . Let $\epsilon = 1/\kappa$. Under the constraint $\deg(g, \partial D) = d$, a minimizer ψ_ϵ must have at least $|d|$ zeros. The leading order of the energy around each vortex is estimated as $2\pi \log(1/\epsilon)$. The result of Bethuel *et al.* (1994) describes the energy for a minimizer

$$G(\psi_\epsilon) = 2\pi|d| \log(1/\epsilon) + \gamma + W(a_1^\epsilon, \dots, a_{|d|}^\epsilon) + o(1)$$

where $\{a_j^\epsilon\}$ are zeros of ψ_ϵ and γ is a universal constant. The function W is explicitly given as

$$W(a_1, \dots, a_{|d|}) = 2\pi \sum_{1 \leq j, k \leq |d|, j \neq k} \log |a_j - a_k| + R$$

where R is derived from a Green function satisfying some boundary condition depending on g . Moreover, as $\epsilon \rightarrow 0$, the zeros converge to a minimizer of W , which implies that the asymptotic position of every zero (vortex) is determined by the explicit function W . The first term of W shows that vortices with the same sign of the degree are repulsive to one another and the optimal arrangement of vortices never allows the superposition of multivortices. Although the boundary condition is rather artificial, their mathematical formulation promoted the development of variational methods applied to the Ginzburg–Landau equation.

Time-Dependent Ginzburg–Landau Equations

The Ginzburg–Landau equations in the preceding sections are static models. We consider time evolution models called the time-dependent Ginzburg–Landau equations. The evolution equations serve various numerical simulations exhibiting dynamical properties of solutions. They also provide mathematical problems on global time behaviors of solutions, stability of stationary solutions, dynamical laws of vortices, etc. The Ginzburg–Landau energy is denoted by $\mathcal{E}(u)$, $u = (\Psi, \mathbb{A})$. The simplest model for the time-dependent problem is the gradient flow for $\mathcal{E}(u)$

$$\partial_t u = - \frac{\delta \mathcal{E}}{\delta u}$$

where $\delta \mathcal{E}/\delta u$ is the first variation of the energy. A more standard evolution equation in a nondimensional form is given by

$$(\partial_t + i\phi)\Psi - D_A^2 \Psi = \kappa^2(1 - |\Psi|^2)\Psi \quad [25]$$

$$\eta(\partial_t \mathbb{A} + \nabla \phi) + \text{curl}^2 \mathbb{A} = \text{Im}(\Psi^* D_A \Psi) + \text{curl} H_{\text{ap}} \quad [26]$$

where $\phi(x, t)$ is the electric (scalar) potential and η is a positive parameter with a physical quantity. In fact, this equation was derived by Gor'kov and Eliashberg from the Bardeen, Cooper, and Schrieffer (BCS) theory.

The system of the equations [25]–[26] is invariant under the following time-dependent gauge transformation:

$$(\Psi, \phi, \mathbb{A}) \mapsto (\Psi \exp(i\chi), \phi - \partial_t \chi, \mathbb{A} + \nabla \chi)$$

The equations in the bounded domain $D \subset \mathbb{R}^2$ are considered—subject to boundary and initial conditions

$$\begin{aligned} D_A \Psi \cdot \mathbf{n} &= 0 && \text{on } \partial\Omega \times (0, T) \\ \operatorname{curl} \mathbf{A} &= H_a && \text{on } \partial\Omega \times (0, T) \\ \Psi(x, 0) &= \Psi_0 && \text{in } \Omega \\ \mathbf{A}(x, 0) &= \mathbf{A}_0(x) && \text{in } \Omega \end{aligned} \quad [27]$$

Then, besides the Coulomb gauge [8], we can choose the Lorentz gauge as follows:

$$\begin{aligned} \operatorname{div} \mathbf{A} + \phi &= 0 && \text{in } D, \quad \int_D \phi \, dx = 0 \\ \mathbf{A} \cdot \mathbf{n} &= 0 && \text{on } \partial D \end{aligned}$$

For a smooth solution $u(x, t)$ to [25]–[26] with [27],

$$\frac{d}{dt} \mathcal{E}(u) = -2 \int_{\Omega} |(\partial_t + i\phi)\Psi|^2 + \eta |\partial_t \mathbf{A} + \nabla \phi|^2 \, dx \leq 0$$

holds if H_{ap} is time independent. This is also true in the case of the whole space \mathbb{R}^2 with a condition for the asymptotic behavior as $|x| \rightarrow \infty$.

Suppose that a domain $\Omega \subset \mathbb{R}^3$ is occupied by a superconducting sample and it is surrounded by a medium (or vacuum). Then the electromagnetic behavior in the outside domain, caused by the induced magnetic field of a supercurrent in Ω and an applied magnetic field, should be expressed by the Maxwell equations. With the electric field $\mathbf{E} = -(\mu \partial_t \mathbf{A} + \nabla \phi)$, we obtain

$$-\nu \partial_t \mathbf{E} - \sigma \mathbf{E} + \operatorname{curl}^2 \mathbf{A} = \operatorname{curl} H_{ap} \quad \text{in } \mathbb{R}^3 \setminus \bar{\Omega}$$

where μ, ν , and σ are physical parameters (e.g., $\sigma = 0$ in the vacuum). To match the inside and the outside of Ω , appropriate boundary conditions are required.

From a point of the gauge theory as in the section “Ginzburg–Landau equations in \mathbb{R}^2 ,” the following time-dependent equations in the whole space are also considered:

$$\begin{aligned} (\partial_t + i\phi)^2 \Psi - D_A^2 \Psi &= \kappa^2 (1 - |\Psi|^2) \Psi \\ -\partial_t \mathbf{E} + \operatorname{curl}^2 \mathbf{A} &= \operatorname{Im}(\Psi^* D_A \Psi) \\ -\nabla \cdot \mathbf{E} &= \operatorname{Im}(\Psi^* (\partial_t + i\phi) \Psi) \end{aligned}$$

Other Topics

In realistic problems, a superconducting sample contains impurities. This inhomogeneity is usually expressed by putting a variable coefficient into the Ginzburg–Landau energy and the equations. Such a model with a variable coefficient is useful in studies for pinning of vortices, Josephson effect through an

inhomogeneous media, etc. A model in a thin film with variable thickness is also described by the Ginzburg–Landau equations with a variable coefficient. Since the Ginzburg–Landau equations (or a modified model) can be considered in various settings, more applications to realistic problems would be treated by the development of nonlinear analysis.

See also: Abelian Higgs Vortices; Bifurcation Theory; Evolution Equations: Linear and Nonlinear; High T_c Superconductor Theory; Image Processing; Mathematics; Integrable Systems: Overview; Interacting Stochastic Particle Systems; Ljusternik–Schnirelman Theory; Nonlinear Schrödinger Equations; Quantum Phase Transitions; Variational Techniques for Ginzburg–Landau Energies.

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Glassy Disordered Systems: Dynamical Evolution

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Introduction

Many macroscopic systems if left to evolve in isolation or in contact with a bath, are able to relax, after a finite time, to history-independent equilibrium states characterized by time-independent values of the state variables and time-translation invariance correlations. In glassy systems, the relaxation time becomes so large that equilibrium behavior is never observed. On short timescales, the microscopic degrees of freedom appear to be frozen in far-from-equilibrium disordered states. On longer timescales slow, history-dependent, off-equilibrium relaxation phenomena become detectable.

The list of physical systems falling in disordered glassy states at low temperature is long, just to mention a few examples one can cite the canonical case of simple and complex liquid systems undergoing a glass transition, polymeric glasses, dipolar glasses, spin glasses, charge density wave systems, vortex systems in type II superconductors, and many other systems.

Experimental and theoretical research has pointed out the existence of dynamical scaling laws characterizing the off-equilibrium evolution of glassy systems. These laws, in turn, reflect the statistical properties of the regions of configuration space explored during relaxation.

The goal of a theory of glassy systems is the comprehension of the mechanisms that lead to the growth of relaxation time and the nature of the scaling laws in off-equilibrium relaxation. A well-developed description of glassy phenomena is provided by mean-field theory based on spin glass models, which gives a coherent framework that is able to describe the dynamics of glassy systems and provides a statistical interpretation of glassy relaxation. Despite important limitations of the mean-field description for finite-dimensional systems, it allows precise discussions of general concepts such as effective temperatures and configurational entropies that have been successfully applied to the description of glassy systems.

In the following, examples of two different ways of freezing will be discussed: spin glasses, where disorder is built in the random nature of the coupling between the dynamical variables, and structural glasses, where the disordered nature of the frozen state has a self-induced character. These systems are examples of two different ways of freezing.

A Glimpse of Freezing Phenomenology

Spin Glasses

The archetypical example of systems undergoing the complex dynamical phenomena described in this article is the case of spin glasses (Fischer and Hertz 1991, Young 1997). Spin glass materials are magnetic systems where the magnetic atoms occupy random position in lattices formed by nonmagnetic matrices fixed at the moment of the preparation of the material. The exchange interaction between the spin of the magnetic impurities in these materials is an oscillating function, taking positive and negative values according to the distance between the atoms.

Spin glass models (see Spin Glasses, Mean Field Spin Glasses and Neural Networks, and Short-Range Spin Glasses: The Metastate Approach) are defined by giving the form of the exchange Hamiltonian, describing the interaction between the spins S_i of the magnetic atoms. In the presence of an external magnetic field h , the exchange Hamiltonian can be written as

$$H = - \sum_{i,j \in \Lambda} J_{ij} S_i \cdot S_j - h \sum_{i \in \Lambda} S_i \quad [1]$$

The spin variable can have classical or quantum nature. This article will be limited to the physics of classical systems. The most common choice in models is to use Ising variables $S_i = \pm 1$. The couplings J_{ij} , which in real material depend on the distance, are most commonly chosen to be independent random variables with a distribution with support on both positive and negative values. Most commonly, one considers either a symmetric bimodal distribution on $\{-1, 1\}$ or a symmetric Gaussian. The sums are restricted to lattices Λ of various types. The most common choices are $\Lambda = \mathbb{Z}^d$ for the Edwards–Anderson model, the complete graph $\Lambda = \{(i, j) | i < j; i, j = 1, \dots, N\}$ for the Sherrington–Kirkpatrick (SK) model, and the Erdos–Renyi random graph for the Viana–Bray (VB) model.

The presence of interactions of both signs induces frustration in the system: the impossibility of minimizing all the terms of the Hamiltonian at the same time. One then has a complex energy landscape, where relaxation to equilibrium is hampered by barriers of energetic and entropic nature.

Spin glass materials, which have a paramagnetic behavior at high temperature, show glassy behavior at low temperature, where magnetic degrees of freedom appear to be frozen for long times in apparently random directions. There is quite a

general consensus, based on the analysis of the experimental data and the numerical simulations, that in three dimensions and in the absence of a magnetic field, the two regimes are separated by a thermodynamic phase transition at a temperature T_c where the magnetic response χ exhibits a cusp (see Figure 1). By linear response, χ is related to the equilibrium spin correlation function

$$\chi = \frac{1}{K_B T N} \sum_i (\langle S_i^2 \rangle - \langle S_i \rangle^2)$$

having denoted by $\langle \cdot \rangle$ the Boltzmann–Gibbs average. A cusp in χ indicates a second-order transition where the so-called Edwards–Anderson parameter $q = (1/N) \sum_i \langle S_i \rangle^2$ becomes different from zero, indicating freezing of the spins in random directions. In the presence of a magnetic field, although the low-temperature phenomenology is similar to the one at zero field, the thermodynamic nature of the freezing transition is more controversial. Theoretically, mean-field theory, based on the SK model, predicts a phase transition with a cusp in the susceptibility both in the absence and in the presence of a magnetic field. Unfortunately, no firm theoretical result is available on the existence and the nature of phase transitions in finite-dimensional spin glass models which is a completely open problem.

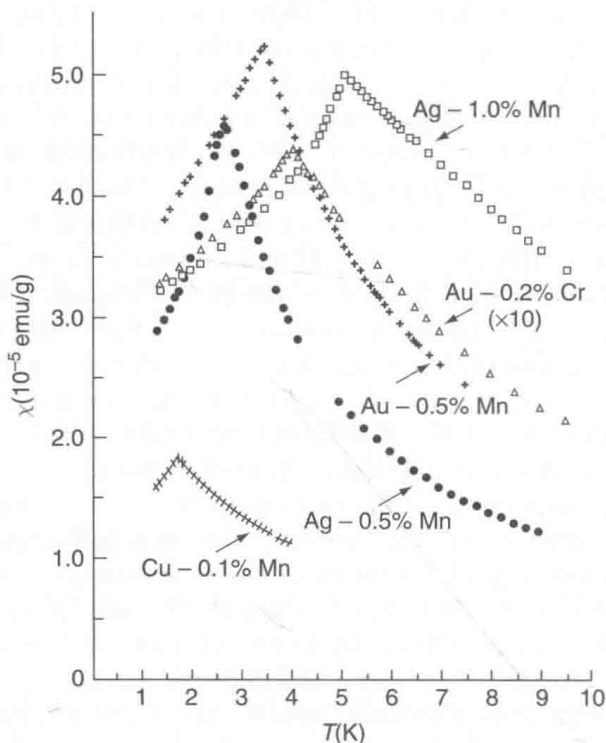


Figure 1 Magnetic susceptibility as a function of temperature in spin glass materials. Reproduced from Fischer KH and Hertz JA (1991) *Spin Glasses*. Cambridge, UK: Cambridge University Press.

Structural Glasses

Analogous freezing of dynamical variables is observed in a variety of systems. Some of them share with the spin glasses the presence of quenched disorder; in many others, this feature is absent. This is the case of structural glasses (Debenedetti 1996).

Many liquids under fast enough cooling, instead of crystallizing, as dictated by equilibrium thermodynamics, form glasses. Simple liquids can be modeled as classical systems of particles with pairwise interactions. In the simplest example of a monoatomic liquid, the potential energy of a configuration is then written as

$$V(r_1, \dots, r_N) = \sum_{i < j} \phi(r_i - r_j) \quad [2]$$

In the case of atomic mixtures, the potential ϕ acquires a dependence on the species of the interacting atoms.

Liquids can be characterized as good or bad glass formers depending on the facility by which they form glasses. In good glass formers, in order to avoid crystallization, it is in general sufficient to cross the region around the liquid–crystal transition point fast enough, so that the systems can set in a supercooled liquid metastable equilibrium. On lowering the temperature, the supercooled liquid becomes denser and more viscous while the relaxation time of the system, related to the viscosity through the Maxwell relation $\tau = \eta/G$ (G is the instantaneous shear modulus of the liquid), undergoes a rapid growth. One defines a conventional glass transition temperature T_g as the point where η takes the solid-like value $\eta = 10^{13}$ Poise, corresponding to a relaxation time $\tau \approx 100$ s. After that point, the system falls out of equilibrium; under usual experimental conditions, it does not have the time to adjust to external solicitations and behaves mechanically like a solid. The glass transition temperature is then characterized as the point where the liquid goes out of equilibrium, the relaxation time becomes larger than the external timescale and the positions of the atoms appear as frozen on that scale.

A great effort has been devoted to understand the behavior of the temperature dependence of the relaxation time and the nature of the dynamical processes in supercooled liquids. In deeply supercooled liquids, the empirical behavior of the relaxation time ranges from the Arrhenius form for “strong glasses” $\tau \sim \exp(\Delta/T)$ to the Vogel–Fulcher form $\tau(T) \sim \exp(D/(T - T_0))$ for “fragile glasses.” The Vogel–Fulcher law predicts a finite-temperature divergence of the relaxation time at the temperature T_0 . Unfortunately, in typical cases, the T_0 results are

estimated to be 10–15% lower than T_g so that it is not possible to verify the law close enough to T_0 to support the divergent behavior.

As a consequence of freezing, one observes important qualitative changes in the behavior of thermodynamic quantities similar to those encountered in equilibrium phase transitions. In a narrow interval around T_g , specific heat and compressibility undergo jumps from liquid-like values to much lower solid-like values.

Aging and Slow Dynamics

While the crudest picture of the glass transition describes freezing as complete structural arrest, both for the cases where the glass transition is a genuine off-equilibrium phenomenon, as in structural glasses, and in the case where it has a thermodynamical character as in spin glasses, the study of dynamical quantities reveals the existence of persisting, history-dependent, slow relaxation processes in the frozen phase (Norblad and Svendlidh 1997). This is the phenomenon of aging, which is a constitutive feature of the glassy state. Its theoretical analysis occupies a central theoretical role in the comprehension of the way glassy systems explore configuration space. A first characterization of relaxation is given by the behavior of “one-time quantities” like internal energy, density, etc., which slowly evolve in the course of time towards values corresponding to states of lower free energy. More interesting is the behavior of “two-time quantities,” time-dependent correlation functions and responses, which reveal the deep off-equilibrium nature of glassy relaxation. In experimental, numerical, and theoretical studies, a special position is occupied by the linear response function. Using the language of magnetic systems, apt to the spin glasses, one considers the response of the magnetization to an applied magnetic field. To deal with other systems, different conjugated couples of variables are considered and simple changes of language are needed. Linear perturbations allow to reveal the dynamics of the systems without affecting its evolution. Denoting by $M(t)$ the magnetization at a time t and by $h(t')$ the magnetic field at time t' , the instantaneous linear response function is defined as

$$R(t, t') = \left(\frac{\delta M(t)}{\delta h(t')} \right)_{h=0} \quad [3]$$

Measures of the time integral of $R(t, t')$ are commonly performed to reveal the presence of aging in glassy systems. Aging is usually studied observing the dynamics that follows a rapid quench from high

temperature, at an instant that marks the origin of time. One can reconstruct the response function measuring the zero-field-cooled (ZFC) magnetization as the response to a magnetic field acting from a waiting time t_w to the measuring time t ,

$$\chi_{\text{ZFC}}(t, t_w) = \int_{t_w}^t dt' R(t, t') \quad [4]$$

or its complement, the thermoremanent magnetization (TRM) corresponding to the response to a magnetic field acting from the time of the quench up to t_w

$$\chi_{\text{TRM}}(t, t_w) = \int_0^{t_w} dt' R(t, t') \quad [5]$$

In Figure 2, the behavior of the susceptibility χ_{ZFC} is shown as a function of $t - t_w$ in a typical example of aging experiment at low temperature. Out-of-equilibrium behavior is manifest in the dependence of the curves on the waiting time t_w . The relaxation appears slower and slower for larger waiting times, and the t_w dependence does not disappear even for very large times. Two nontrivial dynamical regimes can be identified: a first regime for small $t - t_w$, that is, $t - t_w \ll t_w$ where the relaxation is independent of t_w and a second regime roughly valid for $t - t_w \sim t_w$ where time-translation invariance is manifestly violated. The analysis of experimental and simulation data shows a scale-invariant behavior according to which curves corresponding to different waiting times can be superimposed rescaling the time difference $t - t_w$ with a suitable t_w -dependent relaxation time $\tau(t_w)$. This is a growing function of t_w which seems to diverge for large t_w . Up to the waiting times where it has been possible to test the relation, $\tau(t_w)$ behaves as a power $\tau(t_w) \sim t_w^\alpha$ where in different materials and models, $\alpha = 0.8\text{--}0.9$.

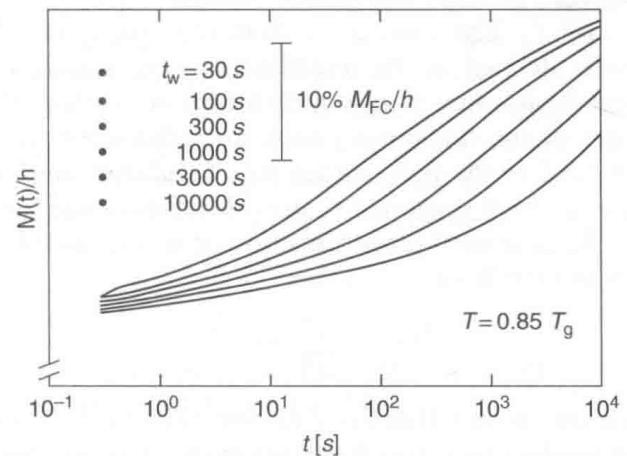


Figure 2 ZFC magnetization in an aging experiment. The curves, from bottom to top, correspond to increasing waiting times. Reproduced from Norblad P and Svendlidh P (1997) Experiments in spin glasses. In: Young AP (ed.) *Spin Glasses and Random Fields*. Singapore: World Scientific, with permission from World Scientific Publishing Co. Pte Ltd.

Many efforts have been devoted to the comprehension of the scaling laws in aging (Bouchaud *et al.*). Among the theories and models of aging that have been proposed, one can cite the phenomenological model known as “trap model,” developed by Bouchaud and collaborators that assimilates aging to a random walk between “traps” characterized by a broad distribution of trapping times. Suitable choices of the trapping-time distribution allow to derive scaling laws similar to the ones characteristic of aging systems. A different theory, the “droplet model” for spin glasses assimilates aging phenomena to the competition between slowly growing domains of equilibrium phases, in analogy with the dynamics of phase separation in first-order phase transitions. The approach that has led to the most detailed and spectacular predictions has been the study of microscopic mean-field models.

Mean-Field Models of Disordered Systems

Mean-field theory starts from the analysis of the relaxation dynamics of disordered systems with weak long-range forces (Bouchaud *et al.*). The reference model of spin glass mean-field theory is the so called p -spin model, which considers N spins S_i with random p -body interactions with each other and is described by the Hamiltonian

$$H_p(S) = \sum_{i_1 < \dots < i_p}^{1,N} J_{i_1, \dots, i_p} S_{i_1} \cdots S_{i_p} \quad [6]$$

where the quenched coupling constants J_{i_1, \dots, i_p} are assumed to be i.i.d. Gaussian variables with zero average and N dependent variance $E(J_{i_1, \dots, i_p}^2) = p!/2N^{p-1}$. The case $p=2$ coincides with the SK model defined in the introduction. The reason for considering the p -spin generalization is that the order of the transition passes from the second one for $p=2$ to the first one for $p \geq 3$ and that this last case has been suggested to provide a mean-field limit for the structural glass transition. It is also useful to define Hamiltonians

$$H[S] = \sum_{p \geq 1} a_p H_p[S] \quad [7]$$

that mix p -spin Hamiltonians for different p . These are random Gaussian functions of the spin variables, with covariance induced by the coupling distribution

$$\begin{aligned} E[H(S)H(S')] &= Nf(q(S, S')) \\ &= \frac{N}{2} \sum_{p \geq 1} a_p^2 q(S, S')^p \end{aligned} \quad [8]$$

where the function

$$q(S, S') = \frac{1}{N} \sum_{i=1}^N S_i S'_i$$

is the overlap between configurations. A crucial hypothesis in the study of relaxation in spin systems is that any local spin update rule verifying the detailed balance condition with respect to the Boltzmann–Gibbs measure gives rise to the same long-time properties. In this perspective, in Monte Carlo simulations, it is convenient to use Ising spins with Metropolis or Glauber dynamics. Much theoretical progress has been achieved considering spherical models where the spin variables are real numbers subject to a global spherical constraint $\sum_i S_i^2 = N$ and evolve according to the following Langevin dynamics:

$$\frac{dS_i(t)}{dt} = -\frac{\partial H(S(t))}{\partial S_i} - \mu(t)S_i(t) + \eta_i(t) \quad [9]$$

where $\mu(t)$ is a time-dependent multiplier that at each instant of time insures that the spherical constraint is respected, and $\eta_i(t)$ is a thermal white noise with variance

$$E(\eta_i(t)\eta_j(s)) = 2T\delta_{ij}\delta(t-s) \quad [10]$$

In order to model the quench from high temperature performed in experiments, the initial conditions are randomly chosen with uniform probability. To describe long but finite-time dynamics, it is necessary to consider the limit of large volume $N \rightarrow \infty$ for finite time, which is the only case where one can have infinite relaxation times. Application of functional Martin–Siggia–Rose techniques has allowed the derivation of closed integro-differential equations for the spin autocorrelation function

$$C(t, t') = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^N \langle S_i(t) S_i(t') \rangle$$

and the response to an impulsive external field

$$h_i(t), R(t, t') = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^N \left\langle \frac{\delta S_i(t)}{\delta h_i(t')} \right\rangle$$

where the average has to be intended on quenched disordered couplings, initial conditions, and realization of thermal noise. Unfortunately, in the case $p=2$ relevant for spin glass phenomenology, the spherical constraints reduce the model to a linear system where different eigenmodes of the interaction matrix J_{ij} evolve independently. This oversimplification renders the model similar to systems apt to describe phase separation rather than freezing phenomena. Many of the glassy features of the SK model however are captured by a mixture of $p=2$

with $p=4$ Hamiltonians and $f(q)=(1/2)(q^2 + aq^4)$. For the general Hamiltonian [7] one gets the coupled equations

$$\begin{aligned} \frac{\partial C(t, t')}{\partial t} &= -\mu(t)C(t, t') \\ &+ \int_0^t dt'' f''(C(t, t''))R(t, t'')C(t', t'') \\ &+ \int_{t'}^t dt'' f'(C(t, t''))R(t'', t') \end{aligned}$$

$$\frac{\partial R(t, t')}{\partial t} = -\mu(t)R(t, t') + \int_{t'}^t dt'' f''(C(t, t''))R(t, t'')R(t'', t') \quad [11]$$

$\mu(t)$ is a multiplier that at each instant of time insures the spherical constraint $C(t, t)=1$, and is determined by

$$\mu(t) = \int_0^t dt'' C(t, t'')R(t, t'') + T \quad [12]$$

In the next sections, we will discuss how these equations describe dynamical freezing at low temperature. The gross features are determined by the form of the function $f(q)$. Two main behaviors can be identified:

1. Systems of type I. This behavior is found if $f'''(q)/(f''(q))^{3/2}$ is a monotonically decreasing function of q . To this family belongs the pure spherical p -spin model for $p \geq 3$, and one finds a dynamical transition not corresponding to a point of singularity in the free energy where the Edwards–Anderson parameter jumps discontinuously to a nonzero value. Models of this family have been proposed as appropriate mean-field limits for structural glass behavior.
2. Systems of type II. This behavior is found if $f'''(q)/(f''(q))^{3/2}$ is a monotonically increasing function of q . This family mimics the behavior of the SK model. An example of function f verifying the condition for type II behavior is $f(q)=1/2(q^2 + aq^4)$ for sufficiently small but positive values of a . In this case, the dynamical transition is found at a point of second-order singularity of the free energy and the Edwards–Anderson parameter is continuous at the transition. Models of this family provide a mean-field limit for spin glass type behavior.

Equilibrium Dynamics at High Temperature

At high temperature, after a finite transient, eqn [11] describes equilibrium behavior. In these conditions,

time-translation invariance holds $C(t, t')=C(t-t')$, $R(t, t')=R(t-t')$ while the Lagrange multiplier μ becomes time independent. In addition, correlation and response are related by the fluctuation–dissipation theorem (FDT) relation

$$R(t) = -\frac{1}{T} \frac{dC(t)}{dt} \quad [13]$$

Ergodic behavior is manifest in the fact that the dynamics decorrelate completely; $\lim_{t \rightarrow \infty} C(t)=0$. Then from [11] one gets the equilibrium equation:

$$\frac{dC(t)}{dt} = -TC(t) - \frac{1}{T} \int_0^t ds f'(C(t-s)) \frac{dC(s)}{ds} \quad [14]$$

It is worth noticing that this equation, apart from an irrelevant inertial term, coincides for type I systems with the schematic mode-coupling theory (MCT) equation which has been successfully used to describe moderate supercooled liquids (Goetze 1989). In the context of liquid theory, mode-coupling equations stem from an approximate treatment for the dynamical evolution of the density–density space and time-dependent correlation function. The schematic MCT equations consider an equation for a single mode, neglecting any space dependence of the correlator.

Both in type I and in type II systems, eqn [14] displays a dynamical transition at a finite temperature T_c where the relaxation time diverges as a power law $\tau \sim |T - T_c|^{-\epsilon}$ and the asymptotic value of the correlation acquires a nonzero value.

This behavior in type I systems represents a failure of MCT to describe the temperature dependence of the relaxation time in supercooled liquids, which, as previously observed, empirically follows the Vogel–Fulcher law. The MCT temperature is interpreted as a singularity which is avoided in supercooled liquids, thanks to relaxation mechanisms specific of short-range systems. It has been noticed that this singularity at T_c can be associated to the growth of spatial heterogeneities and dynamical correlations, as exemplified in the behavior of the four-point function

$$\chi_4(t) = \frac{1}{N} \sum_{i,j} \langle S_i(t) S_j(t) S_i(0) S_j(0) \rangle$$

and its associate correlation length (Franz and Parisi 2000, Biroli and Bouchaud 2004).

Off-Equilibrium Dynamics Below T_c : Aging and Slow Dynamics

Type I systems Below the transition temperature T_c slow dynamics and aging set in. In 1993, Cugliandolo and Kurchan found a long-time

solution to the equations of motion [11] for type I systems describing an asymptotic off-equilibrium state that follows from high-temperature quench. Soon after, type II systems were also analyzed (Bouchaud *et al.*).

The equations can be analyzed in the limit in which both times tend to infinity $t, t' \rightarrow \infty$. In this regime all “one-time quantities,” that is, state functions like energy, magnetization, etc., reach asymptotic time-independent limit. Though the decay to the asymptotic value cannot read directly from the analysis of the equations in that limit, numerical and theoretical evidence suggests that the final values are approached as power laws in time.

The study of correlation and response functions displays an asymptotic scaling behavior similar to the one observed in glassy systems in laboratory and numerical experiments.

Two different interesting regimes are found, first of all there is a stationary regime: the limit $t, t_w \rightarrow \infty$ is performed keeping the difference $t - t_w = s$ finite. In this regime, equilibrium behavior is observed, with correlation and response related by the FDT relation $R_{st}(s) = -\beta \partial C_{st}(s) / \partial s$. The stationary regime is followed by an aging regime, where correlations decay below the value $q_{EA} = \lim_{s \rightarrow \infty} C_{st}(s)$ down to zero. One of the most striking features of aging evolution is that the system – though at a decreasing speed – constantly move far apart from any visited region of configuration space. The decay of correlations is nonstationary and takes place on a timescale $\tau(t_w)$ diverging for large t_w . While the theory can infer the existence of the timescale $\tau(t_w)$, its precise form remains undetermined. This is a consequence of an asymptotic invariance under monotonous time reparametrizations $t \rightarrow g(t)$ appearing for large times. Coherently with nonstationary behavior, other equilibrium properties break down in the aging regime. Correlation and response which do not verify the FDT are rather asymptotically related by a generalized form of the fluctuation–dissipation relation

$$R_{ag}(t, t_w) = \frac{X}{T} \frac{\partial C_{ag}((t - t_w)/\tau(t_w))}{\partial t_w} \quad [15]$$

This relation, despite predicting the vanishing of the instantaneous response, implies a finite contribution of the aging dynamics to the value of the integrated ZFC and TRM responses. The constant X , called fluctuation–dissipation ratio (FDR), is a temperature-dependent factor monotonically varying between the values 1 and 0 as the temperature is decreased from T_c down to zero. Violations of the FDT have to be expected in any off-equilibrium regime; however, a constant ratio between response

and derivative of the correlation is very nongeneric. It is of great theoretical importance that the same constant that governs the FDR among spin auto-correlation and magnetic response, also appears in the relation of any other conceivable couple of correlation and conjugated response in the system. Slow dynamics can be interpreted as motion between finite-life metastable states with well-defined free energy f and exponential multiplicity $\exp(N\Sigma(f))$. The FDR verifies the generalized thermodynamic relation

$$\frac{\partial \Sigma}{\partial f} = \frac{X}{T} \quad [16]$$

This relation is in turn intimately related to the possibility of considering the ratio $T_{\text{eff}} = T/X$ as an effective temperature, that governs the heat exchanges among slow degrees of freedom (Cugliandolo *et al.* 1997). Slow degrees of freedom do not exchange heat with the fast ones, but they are in equilibrium between themselves at the temperature T_{eff} . The validity of relation [16] has been put at the basis of a detailed statistical description of the glassy state (Franz and Virasoro 2000, Biroli and Kurchan 2001, Nieuwenhuizen 2000) which assumes that metastable states with equal free energy are encountered with equal probability during the descent to equilibrium. Modified thermodynamic relations follow, that condensate all the dependence on the thermal history in the value of the effective temperature. Given the interest of a thermodynamic description of the glassy state, many numerical studies have addressed the problem of the identification and determination of effective temperatures from the fluctuation–dissipation relations, and its relation with configurational entropy. In Figure 3 the result of a numerical study on a realistic system is presented, verifying relation [15]. Experimental verifications are at the moment starting and new results are waited in the future.

Type II systems In these systems the dynamic transition occurs at the point of thermodynamic singularity, where the Edwards–Anderson parameter becomes nonzero in a second-order fashion. The magnetic susceptibility exhibits a cusp singularity similar to the one found in spin glass materials. Differently from type I systems, one-time quantities tend to their equilibrium values for long times. The off-equilibrium nature of the relaxation shows up in the behavior of correlations and responses, which display aging behavior.

Their behavior generalizes the one found in type I systems, with a more complex pattern of violation

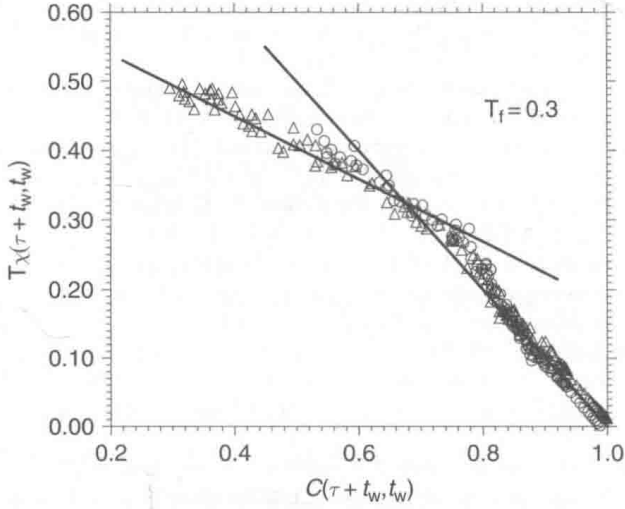


Figure 3 Fluctuation-dissipation plot; $\chi_{ZFC}(t, t_w)$ vs. $C(t, t_w)$ in a model of Lennard-Jones glass for different values of the waiting time t_w . The slope of the curves is equal to the finite-time FDR divided by the temperature. One observes the characteristic shape of type-I systems with an FDR equal to 1 in the stationary regime for high correlations and equal to a constant smaller than 1 in the low-correlations aging regime. Reproduced from Kob W and Barrat J-L (1999) *Europhysics Letters* 46: 637, with permission from EDP Sciences.

of time-translation invariance and FDT. Also in this case a short-time equilibrium behavior can be identified where the correlation decreases from 1 to q_{EA} and a long-time inhomogeneous aging behavior where correlations decrease to zero. Differently from type I system it is impossible to characterize aging through a unique timescale $\tau(t_w)$. One finds instead a continuum of timescales hierarchically organized. The analysis of the equations at the reparametrization-invariant level reveals the existence of a continuum of separate timescales $\tau(t_w, q)$ associated to each value of $C(t, t_w) = q < q_{EA}$ and that $\lim_{t_w \rightarrow \infty} \tau(t_w, q) / \tau(t_w, q') = 0$ for $q > q'$, meaning that for finite t_w the time to decay to q' is much larger than the time to decay to q . For large times, $1 \ll t_1 \ll t_2 \ll t_3$, the correlations verify the ultrametric property $C(t_3, t_1) = \min[C(t_3, t_2), C(t_2, t_1)]$. To each time-scale corresponds in this case a different effective temperature, and correlation and response are related by the equation

$$\beta X(q) = \lim_{\substack{t, t_w \rightarrow \infty \\ C(t, t') = q}} \frac{R(t, t')}{\partial C(t, t') / \partial t'} \quad [17]$$

where the function $X(q)$ is an increasing function of q with the properties of a cumulative probability distribution. In fact it can be seen (Franz *et al.* 1999) that this is related to the Parisi overlap probability function describing the correlations among ergodic components at equilibrium, in a generalization of relation [14]. Figure 4 shows the result of a

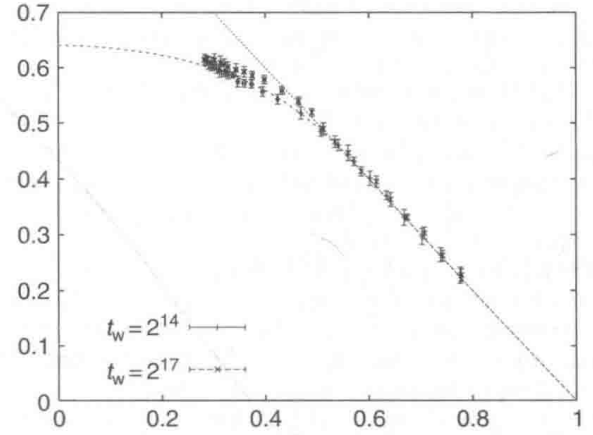


Figure 4 Fluctuation-dissipation plot in a three-dimensional spin glass at low temperature. As predicted for type-II systems, the FDR is an increasing function of the correlation, constant only in the stationary part of the relaxation. Reproduced from Marinari E *et al.* (1998) Violation of the fluctuation dissipation theorem in finite dimensional spin glasses. *Journal of Physics A: Mathematical and General* 31: 2611, with permission from Institute of Physics Publishing Ltd.

numerical experiment in a three-dimensional spin glass, where $X(q)$ is not piecewise constant.

The ideas presented in this article, fruits of mean-field theory of disordered systems, are objects of intense debate in their application to the physics of short-range systems. Many of the relations derived have stimulated a lot of numerical, experimental, and theoretical work. Some of the predictions of the theory are very well verified in many short-range glassy systems, at least on the accessible timescales. Notably, the violations of FDR, and the possibility to associate the values of the FDR to effective temperatures is very well verified both in structural glass models, and in finite-range spin glasses. Since finite aging times imply finite length scales over which the dynamic variables can exhibit correlated behavior, this indicates that the mean-field theory is at least good at describing glassy phenomena on a local scale. The question if the mean-field theory also gives a good description on the infinite time limit and the anomalous response persists forever is at present an open theoretical problem. It relates to the possibility of having mean-field type of equilibrium ergodicity breaking, which is an open question, object of active research.

See also: Interacting Stochastic Particle Systems; Short-Range Spin Glasses: The Metastate Approach; Spin Glasses.

Further Reading

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Graded Poisson Algebras

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Definitions

Graded Vector Spaces

By a \mathbb{Z} -graded vector space (or simply, graded vector space) we mean a direct sum $A = \bigoplus_{i \in \mathbb{Z}} A_i$ of vector spaces over a field k of characteristic zero. The A_i are called the components of A of degree i and the degree of a homogeneous element $a \in A$ is denoted by $|a|$. We also denote by $A[n]$ the graded vector space with degree shifted by n , namely $A[n] = \bigoplus_{i \in \mathbb{Z}} (A[n])_i$ with $(A[n])_i = A_{i+n}$. The tensor product of two graded vector spaces A and B is again a graded vector space whose degree r component is given by $(A \otimes B)_r = \bigoplus_{p+q=r} A_p \otimes B_q$.

The symmetric and exterior algebras of a graded vector space A are defined, respectively, as $S(A) = T(A)/I_S$ and $\bigwedge(A) = T(A)/I_\Lambda$, where $T(A) = \bigoplus_{n \geq 0} A^{\otimes n}$ is the tensor algebra of A and I_S (resp. I_Λ) is the two-sided ideal generated by elements of the form $a \otimes b - (-1)^{|a||b|} b \otimes a$ (resp. $a \otimes b + (-1)^{|a||b|} b \otimes a$), with a and b homogeneous elements of A . The images of $A^{\otimes n}$ in $S(A)$ and $\bigwedge(A)$ are denoted by $S^n(A)$ and $\bigwedge^n(A)$, respectively. Notice that there is a canonical decalage isomorphism $S^n(A[1]) \simeq \bigwedge^n(A)[n]$.

Graded Algebras and Graded Lie Algebras

We say that A is a graded algebra (of degree zero) if A is a graded vector space endowed with a degree zero bilinear associative product: $A \otimes A \rightarrow A$. A graded algebra is graded commutative if the product satisfies the condition

$$a \cdot b = (-1)^{|a||b|} b \cdot a$$

for any two homogeneous elements $a, b \in A$ of degree $|a|$ and $|b|$, respectively.

A graded Lie algebra of degree n is a graded vector space A endowed with a graded Lie bracket on $A[n]$. Such a bracket can be seen as a degree $-n$ Lie bracket on A , that is, as a bilinear operation $\{\cdot, \cdot\}: A \otimes A \rightarrow A[-n]$ satisfying graded antisymmetry and graded Jacobi relations:

$$\{a, b\} = -(-1)^{(|a|+n)(|b|+n)} \{b, a\}$$

$$\{a, \{b, c\}\} = \{\{a, b\}, c\} + (-1)^{(|a|+n)(|b|+n)} \{a\{b, c\}\}$$

Graded Poisson Algebras

We can now define the main object of interest of this note:

Definition 1 A graded Poisson algebra of degree n , or n -Poisson algebra, is a triple $(A, \cdot, \{\cdot, \cdot\})$ consisting of a graded vector space $A = \bigoplus_{i \in \mathbb{Z}} A_i$ endowed with a degree zero graded commutative product and with

a degree $-n$ Lie bracket. The bracket is required to be a biderivation of the product, namely:

$$\{a, b \cdot c\} = \{a, b\} \cdot c + (-1)^{|b|(|a|+n)} b \cdot \{a, c\}$$

Notation. Graded Poisson algebras of degree zero are called Poisson algebras, while for $n=1$ one speaks of Gerstenhaber (1963) algebras or of Schouten algebras.

Sometimes a \mathbb{Z}_2 -grading is used instead of a \mathbb{Z} -grading. In this case, one just speaks of even and odd Poisson algebras.

Example 1 Any graded commutative algebra can be seen as a Poisson algebra with the trivial Lie structure, and any graded Lie algebra can be seen as a Poisson algebra with the trivial product.

Example 2 The most classical example of a Poisson algebra (already considered by Poisson himself) is the algebra of smooth functions on \mathbb{R}^{2n} endowed with usual multiplication and with the Poisson bracket $\{f, g\} = \partial_{q^i} f \partial_{p_i} g - \partial_{q^i} g \partial_{p_i} f$, where the p_i 's and the q^i 's, for $i=1, \dots, n$, are coordinates on \mathbb{R}^{2n} . The bivector field $\partial_{q^i} \wedge \partial_{p_i}$ is induced by the symplectic form $\omega = dp_i \wedge dq^i$. An immediate generalization of this example is the algebra of smooth functions on a symplectic manifold $(\mathbb{R}^{2n}, \omega)$ with the Poisson bracket $\{f, g\} = \omega^{ij} \partial_i f \partial_j g$, where $\omega^{ij} \partial_i \wedge \partial_j$ is the bivector field defined by the inverse of the symplectic form $\omega = \omega_{ij} dx^i \wedge dx^j$; viz. $\omega_{ij} \omega^{jk} = \delta_i^k$.

A further generalization is when the bracket on $C^\infty(\mathbb{R}^m)$ is defined by $\{f, g\} = \alpha^{ij} \partial_i f \partial_j g$, with the matrix function α not necessarily nondegenerate. The bracket is Poisson if and only if α is skewsymmetric and satisfies

$$\alpha^{ij} \partial_i \alpha^{kl} + \alpha^{il} \partial_i \alpha^{jk} + \alpha^{ik} \partial_i \alpha^{lj} = 0$$

An example of this, already considered by Lie (1894), is $\alpha^{ij}(x) = f_k^{ij} x^k$, where the f_k^{ij} 's are the structure constants of some Lie algebra.

Example 3 Example 2 can be generalized to any symplectic manifold (M, ω) . To every function $h \in C^\infty(M)$ one associates the Hamiltonian vector field X_h which is the unique vector field satisfying $i_{X_h} \omega = dh$. The Poisson bracket of two functions f and g is then defined by

$$\{f, g\} = i_{X_f} i_{X_g} \omega$$

In local coordinates, the corresponding Poisson bivector field is related to the symplectic form as in Example 2.

A generalization is the algebra of smooth functions on a manifold M with bracket $\{f, g\} = \langle \alpha | df \wedge dg \rangle$, where α is a bivector field

(i.e., a section of $\wedge^2 TM$) such that $\{\alpha, \alpha\}_{SN} = 0$, where $\{\cdot, \cdot\}_{SN}$ is the Schouten–Nijenhuis bracket (see the first subsection in the next section for details, and Example 2 for the local coordinate expression). Such a bivector field is called a Poisson bivector field and the manifold M is called a Poisson manifold. Observe that a Poisson algebra structure on the algebra of smooth functions on a smooth manifold is necessarily defined this way. In the symplectic case, the bivector field corresponding to the Poisson bracket is the inverse of the symplectic form (regarded as a bundle map $TM \rightarrow T^*M$).

The linear case described at the end of Example 2 corresponds to $M = \mathfrak{g}^*$ where \mathfrak{g} is a (finite-dimensional) Lie algebra. The Lie bracket $\wedge^2 \mathfrak{g} \rightarrow \mathfrak{g}$ is regarded as an element of $\mathfrak{g} \otimes \wedge^2 \mathfrak{g}^* \subset \Gamma(\wedge^2 T\mathfrak{g}^*)$ and reinterpreted as a Poisson bivector field on \mathfrak{g} . The Poisson algebra structure restricted to polynomial functions is described at the beginning of the next section.

Batalin–Vilkovisky Algebras

When n is odd, a generator for the bracket of an n -Poisson algebra A is a degree $-n$ linear map from A to itself,

$$\Delta : A \rightarrow A[-n]$$

such that

$$\Delta(a \cdot b) = \Delta(a) \cdot b + (-1)^{|a|} a \cdot \Delta(b) + (-1)^{|a|} \{a, b\}$$

A generator Δ is called exact if and only if it satisfies the condition $\Delta^2 = 0$, and in this case Δ becomes a derivation of the bracket:

$$\Delta(\{a, b\}) = \{\Delta(a), b\} + (-1)^{|a|+1} \{a, \Delta(b)\}$$

Remark 1 Notice that not every odd Poisson algebra A admits a generator. For instance, a nontrivial odd Lie algebra seen as an odd Poisson algebra with trivial multiplication admits no generator. Moreover, even if a generator Δ for an odd Poisson algebra exists, it is far from being unique. In fact, all different generators are obtained by adding to Δ a derivation of A of degree $-n$.

Definition 2 An n -Poisson algebra A is called an n -Batalin–Vilkovisky algebra, if it is endowed with an exact generator.

Notation. When $n=1$ it is customary to speak of Batalin–Vilkovisky algebras, or simply BV algebras (see Batalin–Vilkovisky Quantization; see also Batalin and Vilkovisky (1963), Getzler (1994), and Koszul (1985)).

There exists a characterization of n -Batalin–Vilkovisky algebras in terms of only the product and the generator (Getzler 1994, Koszul (1985)). Suppose in fact that a graded vector space A is endowed with a degree zero graded commutative product and a linear map $\Delta : A \rightarrow A[-n]$ such that $\Delta^2 = 0$, satisfying the following “seven-term” relation:

$$\begin{aligned} \Delta(a \cdot b \cdot c) + \Delta(a) \cdot b \cdot c + (-1)^{|a|} a \cdot \Delta(b) \cdot c \\ + (-1)^{|a|+|b|} a \cdot b \cdot \Delta(c) \\ = \Delta(a \cdot b) \cdot c + (-1)^{|a|} a \cdot \Delta(b \cdot c) \\ + (-1)^{(|a|+1)|b|} b \cdot \Delta(a \cdot c) \end{aligned}$$

In other words, Δ is a derivation of order 2.

Then, if we define the bilinear operation $\{, \} : A \otimes A \rightarrow A[-n]$ by

$$\begin{aligned} \{a, b\} = (-1)^{|a|} (\Delta(a \cdot b) - \Delta(a) \cdot b \\ - (-1)^{|a|} a \cdot \Delta(b)) \end{aligned}$$

we have that the quadruple $(A, \cdot, \{, \}, \Delta)$ is an n -Batalin–Vilkovisky algebra. Conversely, one easily checks that the product and the generator of an n -Batalin–Vilkovisky algebra satisfy the above “seven-term” relation.

Examples

Schouten–Nijenhuis Bracket

Suppose \mathfrak{g} is a graded Lie algebra of degree zero. Then $A = S(\mathfrak{g}[n])$ is a $(-n)$ -Poisson algebra with its natural multiplication (the one induced from the tensor algebra $T(A)$) and a degree $-n$ bracket defined as follows (Koszul 1985, Krasil’schik 1988): the bracket on $S^1(\mathfrak{g}[n]) = \mathfrak{g}[n]$ is defined as the suspension of the bracket on \mathfrak{g} , while on $S^k(\mathfrak{g}[n])$, for $k > 1$, the bracket, often called the Schouten–Nijenhuis bracket, is defined inductively by forcing the Leibniz rule

$$\{a, b \cdot c\} = \{a, b\} \cdot c + (-1)^{|b|(|a|+n)} b \cdot \{a, c\}$$

Moreover, when n is odd, there exists a generator defined as

$$\begin{aligned} \Delta(a_1 \cdot a_2 \cdots a_k) \\ = \sum_{i < j} (-1)^\epsilon \{a_i, a_j\} \cdot a_1 \cdots \widehat{a_i} \cdots \widehat{a_j} \cdots a_k \end{aligned}$$

where $a_1, \dots, a_k \in \mathfrak{g}$ and $\epsilon = |a_i| + (|a_i| + 1)(|a_1| + \cdots + |a_{i-1}| + i - 1) + (|a_j| + 1)(|a_1| + \cdots + |\widehat{a_i}| + \cdots + |a_{j-1}| + j - 2)$. An easy check shows that $\Delta^2 = 0$, thus $S(\mathfrak{g}[n])$ is an n -Batalin–Vilkovisky algebra for every odd $n \in \mathbb{N}$. For $n = -1$ the Δ -cohomology

on $\bigwedge \mathfrak{g}$ is the usual Cartan–Chevalley–Eilenberg cohomology.

In particular, one can consider the Lie algebra $\mathfrak{g} = \text{Der}(B) = \bigoplus_{j \in \mathbb{Z}} \text{Der}^j(B)$ of derivations of a graded commutative algebra B . More explicitly, $\text{Der}^j(B)$ consists of linear maps $\phi : B \rightarrow B$ of degree j such that $\phi(ab) = \phi(a)b + (-1)^{j|a|} a\phi(b)$ and the bracket is $\{\phi, \psi\} = \phi \circ \psi - (-1)^{|\phi||\psi|} \psi \circ \phi$. The space of multi-derivations $S(\text{Der}(B)[-1])$, endowed with the Schouten–Nijenhuis bracket, is a Gerstenhaber algebra.

We can further specialize to the case when B is the algebra $C^\infty(M)$ of smooth functions on a smooth manifold M ; then $\mathfrak{X}(M) = \text{Der}(C^\infty(M))$ is the space of vector fields on M and $\mathcal{V}(M) = S(\mathfrak{X}(M)[-1])$ is the space of multivector fields on M . It is a classical result by Koszul (1985) that there is a bijective correspondence between generators for $\mathcal{V}(M)$ and connections on the highest exterior power $\bigwedge^{\dim M} TM$ of the tangent bundle of M . Moreover, flat connections correspond to generators which square to zero.

Lie Algebroids

A Lie algebroid E over a smooth manifold M is a vector bundle E over M together with a Lie algebra structure (over \mathbb{R}) on the space $\Gamma(E)$ of smooth sections of E , and a bundle map $\rho : E \rightarrow TM$, called the anchor, extended to a map between sections of these bundles, such that

$$\{X, fY\} = f\{X, Y\} + (\rho(X)f)Y$$

for any smooth sections X and Y of E and any smooth function f on M . In particular, the anchor map induces a morphism of Lie algebras $\rho_* : \Gamma(E) \rightarrow \mathfrak{X}(M)$, namely $\rho_*\{X, Y\} = \{\rho_*(X), \rho_*(Y)\}$.

The link between Lie algebroids and Gerstenhaber algebras is given by the following Proposition (Kosmann-Schwarzbach and Monterde 2002, Xu 1999):

Proposition 1 *Given a vector bundle E over M , there exists a one-to-one correspondence between Gerstenhaber algebra structures on $A = \Gamma(\bigwedge(E))$ and Lie algebroid structures on E .*

The key of the proposition is that one can extend the Lie algebroid bracket to a unique graded antisymmetric bracket on $\Gamma(\bigwedge(E))$ such that $\{X, f\} = \rho(X)f$ for $X \in \Gamma(\bigwedge^1(E))$ and $f \in \Gamma(\bigwedge^0(E))$, and that for $Q \in \Gamma(\bigwedge^{q+1}(E))$, $\{Q, \cdot\}$ is a derivation of $\Gamma(\bigwedge(E))$ of degree q .

Example 4 A finite-dimensional Lie algebra \mathfrak{g} can be seen as a Lie algebroid over a trivial base manifold. The corresponding Gerstenhaber algebra is the one of last subsection.

Example 5 The tangent bundle TM of a smooth manifold M is a Lie algebroid with anchor map given by the identity and algebroid Lie bracket given by the usual Lie bracket on vector fields. In this case, we recover the Gerstenhaber algebra of multi-vector fields on M described in the last subsection.

Example 6 If M is a Poisson manifold with Poisson bivector field α , then the cotangent bundle T^*M inherits a natural Lie algebroid structure where the anchor map $\alpha^\# : T_p^*M \rightarrow T_pM$ at the point $p \in M$ is given by $\alpha^\#(\xi)(\eta) = \alpha(\xi, \eta)$, with $\xi, \eta \in T_p^*M$, and the Lie bracket of the 1-forms ω_1 and ω_2 is given by

$$\{\omega_1, \omega_2\} = L_{\alpha^\#(\omega_1)}\omega_2 - L_{\alpha^\#(\omega_2)}\omega_1 - d\alpha(\omega_1, \omega_2)$$

The associated Gerstenhaber algebra is the de Rham algebra of differential forms endowed with the bracket defined by Koszul (1985). As shown in Kosmann-Schwarzbach (1995), $\Gamma(\wedge(T^*M))$ is indeed a BV algebra with an exact generator $\Delta = [d, i_\alpha]$ given by the commutator of the contraction i_α with the Poisson bivector α and the de Rham differential d . Similar results hold if M is a Jacobi manifold.

It is natural to ask what additional structure on a Lie algebroid E makes the Gerstenhaber algebra $\Gamma(\wedge(E))$ into a BV algebra. The answer is given by the following result, which is proved in Xu (1999).

Proposition 2 *Given a Lie algebroid E , there is a one-to-one correspondence between generators for the Gerstenhaber algebra $\Gamma(\wedge(E))$ and E -connections on $\wedge^{\text{rk} E} E$ (where $\text{rk} E$ denotes the rank of the vector bundle E). Exact generators correspond to flat E -connections, and in particular, since flat E -connections always exist, $\Gamma(\wedge(E))$ is always a BV algebra.*

Lie Algebroid Cohomology

A Lie algebroid structure on $E \rightarrow M$ defines a differential δ on $\Gamma(\wedge E^*)$ by

$$\delta f := \rho^* df, \quad f \in C^\infty(M) = \Gamma(\wedge^0 E^*)$$

and

$$\begin{aligned} \langle \delta \alpha, X \wedge Y \rangle &:= \langle \delta \langle \alpha, X \rangle, Y \rangle - \langle \delta \langle \alpha, Y \rangle, X \rangle \\ &\quad - \langle \alpha, \{X, Y\} \rangle X, Y \in \Gamma(E), \alpha \in \Gamma(E^*) \end{aligned}$$

where $\rho^* : \Omega^1(M) \rightarrow \Gamma(E^*)$ is the transpose of $\rho_* : \Gamma(E) \rightarrow \mathfrak{X}(M)$ and \langle, \rangle is the canonical pairing of sections of E^* and E . On $\Gamma(\wedge^n E^*)$, with $n \geq 2$, the differential δ is defined by forcing the Leibniz rule.

In Example 4 we get the Cartan–Chevalley–Eilenberg differential on $\wedge \mathfrak{g}^*$; in Example 5 we recover the de Rham differential on $\Omega^*(M) = \Gamma(\wedge T^*M)$, while in Example 6 the differential on $\mathcal{V}(M) = \Gamma(\wedge TM)$ is $\{\alpha, \}_\text{SN}$.

Lie–Rinehart Algebras

The algebraic generalization of a Lie algebroid is a Lie–Rinehart algebra. Recall that given a commutative associative algebra B (over some ring R) and a B -module \mathfrak{g} , then a Lie–Rinehart algebra structure on (B, \mathfrak{g}) is a Lie algebra structure (over R) on \mathfrak{g} and an action of \mathfrak{g} on the left on B by derivations, satisfying the following compatibility conditions:

$$\begin{aligned} \{\gamma, a\sigma\} &= \gamma(a)\delta + a\{\gamma, \sigma\} \\ (a\gamma)(b) &= a(\gamma(b)) \end{aligned}$$

for every $a, b \in B$ and $\gamma, \sigma \in \mathfrak{g}$.

The Lie–Rinehart structures on the pair (B, \mathfrak{g}) bijectively correspond to the Gerstenhaber algebra structures on the exterior algebra $\wedge_B(\mathfrak{g})$ of \mathfrak{g} in the category of B -modules. When \mathfrak{g} is of finite rank over B , generators for these structures are in turn in bijective correspondence with (B, \mathfrak{g}) -connections on $\wedge_B^{\text{rk} \mathfrak{g}} B^{\mathfrak{g}}$, and flat connections correspond to exact generators. For additional discussions, see Gerstenhaber and Schack (1992) and Huebschmann (1998).

Lie algebroids are Lie–Rinehart algebras in the smooth setting. Namely, if $E \rightarrow M$ is a Lie algebroid, then the pair $(C^\infty(M), \Gamma(E))$ is a Lie–Rinehart algebra (with action induced by the anchor and the given Lie bracket).

Lie–Rinehart Cohomology

Lie algebroid cohomology may be generalized to every Lie–Rinehart algebra (B, \mathfrak{g}) . Namely, on the complex $\text{Alt}_B(\mathfrak{g}, B)$ of alternating multilinear functions on \mathfrak{g} with values in B , one can define a differential δ by the rules

$$\begin{aligned} \langle \delta a, \gamma \rangle &= \gamma(a), \quad a \in B = \text{Alt}_B^0(\mathfrak{g}, B), \quad \gamma \in \mathfrak{g} \\ \langle \delta a, \gamma \wedge \sigma \rangle &= \langle \delta \langle a, \gamma \rangle, \sigma \rangle - \langle \delta \langle a, \sigma \rangle, \gamma \rangle - \langle a, \{\gamma, \sigma\} \rangle \\ \gamma, \sigma &\in \mathfrak{g}, \quad a \in \text{Alt}_B^1(\mathfrak{g}, B) \end{aligned}$$

and forcing the Leibniz rule on elements of $\text{Alt}_B^n(\mathfrak{g}, B)$, $n \geq 2$.

Hochschild Cohomology

Let A be an associative algebra with product μ , and consider the Hochschild cochain complex $\text{Hoch}(A) = \prod_{n \geq 0} \text{Hom}(A^{\otimes n}, A)[-n+1]$. There are two basic operations between two elements $f \in \text{Hom}(A^{\otimes k}, A)[-k+1]$ and $g \in \text{Hom}(A^{\otimes l}, A)[-l+1]$, namely a degree zero product

$$\begin{aligned} f \cup g &(a_1 \otimes \cdots \otimes a_{k+l}) \\ &= (-1)^{kl} f(a_1 \otimes \cdots \otimes a_l) \cdot g(a_{l+1} \otimes \cdots \otimes a_{k+l}) \end{aligned}$$

and a degree -1 bracket $\{f, g\} = f \circ g - (-1)^{(k-1)(l-1)} g \circ f$, where

$$\begin{aligned} f \circ g(a_1 \otimes \cdots \otimes a_{k+l-1}) \\ = \sum_{i=1}^{k-1} (-1)^{i(l-1)} f(a_1 \otimes \cdots \otimes a_i \otimes g(a_{i+1} \\ \otimes \cdots \otimes a_l)) \otimes \cdots \otimes a_{k+l-1} \end{aligned}$$

It is well known from Gerstenhaber (1963) that the cohomology $\mathbf{HHoch}(A)$ of the Hochschild complex with respect to the differential $d_{\text{Hoch}} = \{\mu, \cdot\}$ has the structure of a Gerstenhaber algebra. More generally, there is a Gerstenhaber algebra structure on Hochschild cohomology of differential graded associative algebras (Loday 1998).

Graded Symplectic Manifolds

The construction of Example 3 can be extended to graded symplectic manifolds (see Supermanifolds; see also Alexandrov *et al.* (1997), Getzler (1994), and Schwarz (1993)). Recall that a symplectic structure of degree n on a graded manifold N is a closed nondegenerate 2-form ω such that $L_E \omega = n\omega$ where L_E is the Lie derivative with respect to the Euler field of N (see Roytenberg (2002) for details). Let us denote by X_h the vector field associated to the function $h \in C^\infty(N)$ by the formula $i_{X_h} \omega = dh$. Then the bracket

$$\{f, g\} = i_{X_f} i_{X_g} \omega$$

gives $C^\infty(N)$ the structure of a graded Poisson algebra of degree n .

If the symplectic form has odd degree and the graded manifold has a volume form, then it is possible to construct an exact generator defined by

$$\Delta(f) = \frac{1}{2} \text{div}(X_f)$$

where div is the divergence operator associated to the given volume form (Getzler 1994, Kosmann-Schwarzbach and Monterde 2002).

An explicit characterization of graded symplectic manifolds has been given in Roytenberg (2002). In particular, it is proved there that every symplectic form of degree n with $n \geq 1$ is necessarily exact. More precisely, one has $\omega = d(i_E \omega / n)$.

Shifted Cotangent Bundles

The main examples of graded symplectic manifolds are given by shifted cotangent bundles. If N is a graded manifold then the shifted cotangent bundle $T^*[n]N$ is the graded manifold obtained by shifting by n the degrees of the fibers of the cotangent bundle of N . This graded manifold possesses a

nondegenerate closed 2-form of degree n , which can be expressed in local coordinates as

$$\omega = \sum_i dx^i \wedge dx_i^\dagger$$

where $\{x^i\}$ are local coordinates on N and $\{x_i^\dagger\}$ are coordinate functions on the fibers of $T^*[n]N$. In local coordinates, the bracket between two homogeneous functions f and g is given by

$$\begin{aligned} \{f, g\} = & -(-1)^{|x_i^\dagger||f|} \frac{\partial f}{\partial x_i^\dagger} \frac{\partial g}{\partial x^i} \\ & - (-1)^{(|f|+n)(|g|+n)+|x_i^\dagger||g|} \frac{\partial g}{\partial x_i^\dagger} \frac{\partial f}{\partial x^i} \end{aligned}$$

If in addition the graded manifold N is orientable, then $T^*[n]N$ has a volume form too; when n is odd, the exact generator $\Delta(f) = (1/2)\text{div} X_f$ is written in local coordinates as

$$\Delta = \frac{\partial}{\partial x_i^\dagger} \frac{\partial}{\partial x^i}$$

In the case $n=1$, we have a natural identification between functions on $T^*[1]N$ and multivector fields $\mathcal{V}(N)$ on N , and we recover again the Gerstenhaber algebra of the subsection “Schouten–Nijenhuis bracket.” Moreover, it is easy to see that, under the above identification, Δ applied to a vector field of N is the usual divergence operator.

Examples from Algebraic Topology

For any $n > 1$, the homology of the n -fold loop space $\Omega^n(M)$ of a topological space M has the structure of an $(n-1)$ -Poisson algebra (May 1972). In particular, the homology of the double loop space $\Omega^2(M)$ is a Gerstenhaber algebra, and has an exact generator defined using the natural circle action on this space (Getzler 1994). The homology of the free loop space $\mathcal{L}(M)$ of a closed oriented manifold M is also a BV algebra when endowed with the “Chas–Sullivan intersection product” and with a generator defined again using the natural circle action on the free loop space (Cohen and Jones 2002).

Applications

BRST Quantization in the Hamiltonian Formalism

The BRST procedure is a method for quantizing classical mechanical systems or classical field theories in the presence of symmetries (see BRST Quantization). The starting point is a symplectic manifold M (the “phase space”), a function H (the “Hamiltonian” of the system) governing the evolution of the system, and the “constraints” given by

several functions g_i which commute with H and among each other up to a $C^\infty(M)$ -linear combination of the g_i 's.

Then the dynamics is constrained on the locus V of common zeros of the g_i 's. When V is a submanifold, the g_i 's are a set of generators for the ideal I of functions vanishing on V . Observe that I is closed under the Poisson bracket. Functions in I are called "first class constraints." The Hamiltonian vector fields of first-class constraints, which by construction tangential to V , are the "symmetries" of the system.

When V is smooth, then it is a coisotropic submanifold of M and the Hamiltonian vector fields determined by the constraints give a foliation \mathcal{F} of V . In the nicest case V is a principal bundle with \mathcal{F} its vertical foliation and the algebra of functions $C^\infty(V/\mathcal{F})$ on the "reduced phase space" (see Poisson Reduction, and Symmetry and Symplectic Reduction) V/\mathcal{F} is identified with the I -invariant subalgebra of $C^\infty(M)/I$.

From a physical point of view, the points of V/\mathcal{F} are the interesting states at a classical level, and a quantization of this system means a quantization of $C^\infty(V/\mathcal{F})$. The BRST procedure gives a method of quantizing $C^\infty(V/\mathcal{F})$ starting from the (known) quantization of $C^\infty(M)$. Notice that these notions immediately generalize to graded symplectic manifolds.

From an algebraic point of view, one starts with a graded Poisson algebra P and a multiplicative ideal I which is closed under the Poisson bracket. The algebra of functions on the "reduced phase space" is replaced by $(P/I)^I$, the I -invariant subalgebra of P/I . This subalgebra inherits a Poisson bracket even if P/I does not. Moreover, the pair $(B, g) = (P/I, I/I^2)$ inherits a graded Lie-Rinehart structure. The "Rinehart complex" $\text{Alt}_{P/I}(I/I^2, P/I)$ of alternating multilinear functions on I/I^2 with values in P/I , endowed with the differential described in the subsection "Lie-Rinehart cohomology," plays the role of the de Rham complex of vertical forms on V with respect to the foliation \mathcal{F} determined by the constraints.

In case V is a smooth submanifold, we also have the following geometric interpretation: let N^*V denote the conormal bundle of V (i.e., the annihilator of TV in T^*P). This is a Lie subalgebroid of T^*P if and only if V is coisotropic. Since we may identify I/I^2 with sections of N^*C (by the de Rham differential), $(P/I, I/I^2)$ is the corresponding Lie-Rinehart pair. The Rinehart complex is then the corresponding Lie algebroid complex $\Gamma(\wedge(N^*V)^*)$ with differential described in the subsection "Lie algebroid cohomology." The image of the anchor map $N^*V \rightarrow TV$ is the distribution determining \mathcal{F} , so by duality we get an injective chain map from the vertical de Rham complex to the Rinehart complex.

The main point of the BRST procedure is to define a chain complex $C^\bullet = \wedge(\Psi^* \oplus \Psi) \otimes P$, where Ψ is a graded vector space, with a coboundary operator D (the "BRST operator"), and a quasi-isomorphism (i.e., a chain map that induces an isomorphism in cohomology)

$$\pi : (C^\bullet, D) \rightarrow (\text{Alt}_{P/I}(I^2/I, P/I), d)$$

This means in particular that the zeroth cohomology $H_D^0(C)$ gives the algebra $(P/I)^I$ of functions on the "reduced phase space." Observe that there is a natural symmetric inner product on $\Psi^* \oplus \Psi$ given by the evaluation of Ψ^* on Ψ . This inner product, as an element of $S^2(\Psi \oplus \Psi^*) \simeq S^2(\Psi) \oplus (\Psi \otimes \Psi^*) \oplus S^2(\Psi^*)$, is concentrated in the component $\Psi \otimes \Psi^*$, and so it defines an element in $\wedge^2(\Psi[1] \oplus \Psi^*[-1]) \simeq S^2(\Psi)[2] \oplus (\Psi \otimes \Psi^*) \oplus S^2(\Psi^*)[-2]$, that is, a degree zero bivector field on $\Psi[1] \oplus \Psi^*[-1]$. It is easy to see that this bivector field induces a degree zero Poisson structure on $S(\Psi^*[-1] \oplus \Psi[1])$. From another viewpoint this is the Poisson structure corresponding to the canonical symplectic structure on $T^*\Psi[1]$. Finally, we have that $S(\Psi^*[-1] \oplus \Psi[1]) \otimes P$ is a degree zero Poisson algebra. Note that the superalgebra underlying the graded algebra $S(\Psi^*[-1] \oplus \Psi[1]) \otimes P$ is canonically isomorphic to the complex $C^\bullet = \wedge(\Psi^* \oplus \Psi) \otimes P$. When $P = C^\infty(M)$, we can think of $S(\Psi^*[-1] \oplus \Psi[1]) \otimes C^\infty(M)$ as the algebra of functions on the graded symplectic manifold $N = (\Psi[1] \oplus \Psi^*[-1]) \times M$ (the "extended phase space"). In physical language, coordinate functions on $\Psi[1]$ are called "ghost fields" while coordinate functions on $\Psi^*[-1]$ are called "ghost momenta" or, by some authors, "antighost fields" (not to be confused with the antighosts of the Lagrangian functional-integral approach to quantization).

Suppose now that there exists an element $\Theta \in S(\Psi^*[-1] \oplus \Psi[1]) \otimes P$ such that $\{\Theta, \cdot\} = D$, that one can extend the "known" quantization of P to a quantization of $S(\Psi^*[-1] \oplus \Psi[1]) \otimes P$ as operators on some (graded) Hilbert space \mathcal{T} and that the operator Q which quantizes Θ has square zero. Then one can consider the "true space of physical states" $H_Q^0(\mathcal{T})$ on which the ad_Q -cohomology of operators will act. This provides one with a quantization of $(P/I)^I$.

For further details on this procedure, and in particular for the construction of D , we refer to Henneaux and Teitelboim (1992), Kostant and Sternberg (1987), and Stasheff (1997), and references therein. Observe that some authors refer to this method as BVF (Batalin-Vilkovisky-Fradkin) and reserve the name BRST for the case when the g_i 's are the components of an equivariant moment map.

For a generalization to graded manifolds different from $(\Psi[1] \oplus \Psi^*[-1]) \times M$ we refer to Roytenberg (2002). There it is proved that the element Θ exists if the graded symplectic form has degree different from -1 .

BV Quantization in the Lagrangian Formalism

The BV formalism (see Batalin–Vilkovisky Quantization; see also Batalin and Vilkovisky (1983) and Henneaux and Teitelboim (1992)) is a procedure for the quantization of physical systems with symmetries in the Lagrangian formalism. As a first step, the “configuration space” M of the system is augmented by the introduction of “ghosts.” If G is the group of symmetries, this means that one has to consider the graded manifold $W = \mathfrak{g}[1] \times M$. The second step is to double this space by introducing “antifields for fields and ghosts,” namely one has to consider the “extended configuration space” $T^*[-1]W$, whose space of functions is a BV algebra (see the subsection “Shifted cotangent bundle.” The algebra of “observables” is by definition the cohomology $H_{\Delta}^*(C^{\infty}(T^*[-1]W))$ with respect to the exact generator Δ .

Related Topics

AKSZ

The graded manifold $T^*[-1]W$ considered above is a particular example of a QP -manifold, that is, of a graded manifold M endowed with an integrable (i.e., self-commuting) vector field Q of degree 1 and a graded Q -invariant symplectic structure P . In quantization of classical mechanical theories, the graded symplectic manifold of interest is the space of fields and antifields with symplectic form of degree 1, while Q is the Hamiltonian vector field defined by the action functional S ; the integrability of Q is equivalent to the classical master equation $\{S, S\} = 0$ for the action functional. Quantization of the theory is then reduced to the computation of the functional integral $\int_{\mathcal{L}} \exp(iS/\hbar)$, where \mathcal{L} is a Lagrangian submanifold of M . This functional integral actually depends only on the homology class of the Lagrangian. Locally, a QP manifold is a shifted cotangent bundle $T^*[-1]N$ and a Lagrangian submanifold is the graph of an exact 1-form. In the notations of the subsection “Shifted cotangent bundle,” a Lagrangian submanifold \mathcal{L} is therefore locally defined by equations $x_i^{\dagger} = \partial\Phi/\partial x^i$, and the function Φ is called a gauge-fixing fermion. The action functional of interest is then the gauge-fixed action $S|_{\mathcal{L}} = S(x^i, \partial\Phi/\partial x^i)$.

The language of QP manifolds has powerful applications to sigma models (see Topological Sigma Models): if Σ is a finite-dimensional graded manifold equipped with a volume element, and M is a QP

manifold, then the graded manifold $C^{\infty}(\Sigma, M)$ of smooth maps from Σ to M has a natural structure of QP manifold which describes some field theory if one arranges for the symplectic structure to be of degree 1. As an illustrative example, if $\Sigma = T[1]X$, for a compact oriented three-dimensional smooth manifold X , and $M = \mathfrak{g}[1]$, where \mathfrak{g} is the Lie algebra of a compact Lie group, the QP manifold $C^{\infty}(\Sigma, M)$ is relevant to Chern–Simons theory on X . Similarly, if $\Sigma = T[1]X$, for a compact oriented two-dimensional smooth manifold X and $M = T[1]N$ is the shifted tangent bundle of a symplectic manifold, then the QP structure on $C^{\infty}(\Sigma, M)$ is related to the A-model with target N ; if the symplectic manifold N is of the form $N = T^*K$ for a complex manifold K , then one can endow $C^{\infty}(\Sigma, M)$ with a complex QP manifold structure, which is related to the B-model with target K ; this shows that, in some sense, the B-model can be obtained from the A-model by “analytic continuation” (Alexandrov *et al.* 1997). If $\Sigma = T[1]X$, for a compact oriented two-dimensional smooth manifold X and $M = T^*[1]N$ with canonical symplectic structure, then the QP structure on $C^{\infty}(\Sigma, M)$ is related to the Poisson sigma model (QP structures on $T^*[1]N$ with canonical symplectic structure are in one-to-one correspondence with Poisson structures on N). The study of QP manifolds is sometimes referred to as “the AKSZ formalism”. In Roytenberg (2002) QP manifolds with symplectic structure of degree 2 are studied and shown to be in one-to-one correspondence with Courant algebroids.

Graded Poisson Algebras from Cohomology of P_{∞}

The Poisson bracket on a Poisson manifold can be derived from the Poisson bivector field α using the Schouten–Nienhuis bracket as follows:

$$\{f, g\} = \{\{\alpha, f\}_{\text{SN}}, g\}_{\text{SN}}$$

This may be generalized to the case of a graded manifold M endowed with a multivector field α of total degree 2 (i.e., $\alpha = \sum_{i=0}^{\infty} \alpha_i$, where α_i is an i -vector field of degree $2 - i$) satisfying the equation $\{\alpha, \alpha\}_{\text{SN}} = 0$. One then has the derived multibrackets

$$\begin{aligned} \lambda_i : A^{\otimes i} &\rightarrow A \\ \lambda_i(a_1, \dots, a_i) &:= \{\{\dots \{\{\alpha_i, a_1\}_{\text{SN}}, a_2\}_{\text{SN}} \dots\}_{\text{SN}}, a_i\}_{\text{SN}} \end{aligned}$$

with $A = C^{\infty}(M)$. Observe that λ_i is a multiderivation of degree $2 - i$. The operations λ_i define the structure of an L_{∞} -algebra on A . Such a structure is called a P_{∞} -algebra (P for Poisson) since the λ_i 's are multiderivations. If $\lambda_0 = \alpha_0$ vanishes, then λ_1 is a differential, and the λ_1 -cohomology inherits a graded Poisson algebra structure. This structure can be used

to describe the deformation quantization of coisotropic submanifolds and to describe their deformation theory.

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See also: Batalin–Vilkovisky Quantization; BRST Quantization; Poisson Reduction; Supermanifolds; Symmetry and Symplectic Reduction; Topological Sigma Models.

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Gravitational Lensing

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Introduction

Einstein's theory of general relativity states that gravity attracts light. The deflection angle of a light ray by an object with mass m was predicted to be

$$\tilde{\alpha} = \frac{4Gm}{c^2 r} \quad [1]$$

where c and G are the velocity of light and the gravitational constant, respectively, and r is the impact parameter. The quantitative measurement of

this light deflection at the solar limb during the solar eclipse in 1919 with

$$\tilde{\alpha} = \frac{4GM_{\odot}}{c^2 R_{\odot}} \approx 1.74 \text{ arcsec} \quad [2]$$

(here m is replaced by the solar mass M_{\odot} and the impact parameter is the solar radius R_{\odot}) confirmed Einstein's theory.

In the decades following this measurement, various aspects of the gravitational lens effect were explored theoretically, which include (1) the possibility of multiple or ring-like images of background sources, (2) the use of lensing as a gravitational telescope on very faint and distant objects, and (3) the possibility of determining Hubble's constant with lensing. Only relatively recently – after the

discovery of the first doubly imaged quasar in 1979 – gravitational lensing became an observational science. Today gravitational lensing is a booming part of astrophysics.

Lensing has established itself as a very useful astrophysical tool with some remarkable successes: with the discovery of multiply-imaged quasars, giant luminous arcs, Einstein rings, quasar and galactic microlensing significant new results in areas as different as cosmology, physics of quasars, and galaxy structure could be reached. In this article, only the aspects of “strong lensing” can be treated. More detailed studies on strong and weak lensing can be found in the “Further reading” section.

Basics of Gravitational Lensing

The path, the size, and the cross section of a light bundle propagating through spacetime in principle are affected by all the matter between the light source and the observer. For most practical purposes, we can assume that the lensing action is dominated by a single matter inhomogeneity at some location between source and observer. This is usually called the “thin-lens approximation”: all the action of deflection is thought to take place at a single distance. This approach is valid only if the relative velocities of lens, source, and observer are small compared to the velocity of light ($v \ll c$) and if the Newtonian potential is small ($|\Phi| \ll c^2$). These two assumptions are justified in all astronomical cases of interest. The size of a galaxy, for example, is of order 50 kpc, even a cluster of galaxies is not much larger than 1 Mpc. This “lens thickness” is small compared to the typical distances of the order of few Gpc between observer and lens or lens and background quasar/galaxy, respectively. We assume that the underlying spacetime is well described by a perturbed Friedmann–Robertson–Walker metric:

$$ds^2 = \left(1 + \frac{2\Phi}{c^2}\right) c^2 dt^2 - a^2(t) \left(1 - \frac{2\Phi}{c^2}\right) d\sigma^2 \quad [3]$$

A detailed description of optics in curved spacetimes and a derivation of the lens equation from Einstein’s field equations can be found in Schneider *et al.* (1992, chapters 3 and 4).

Lens Equation

The basic setup for such a simplified gravitational lens scenario involving a point source and a point lens is displayed in Figure 1. The three ingredients in such a lensing situation are the source S, the lens L, and the observer O. Light rays emitted from the source are deflected by the lens. For a point-like

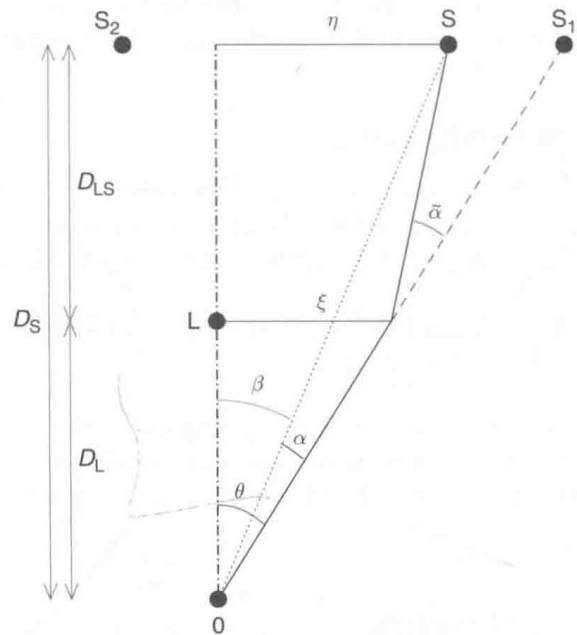


Figure 1 The relation between the various angles and distances involved in the lensing setup can be derived for the case $\tilde{\alpha} \ll 1$ and formulated in the lens equation [6].

lens, there will always be (at least) two images S_1 and S_2 of the source. With external shear – due to the tidal field of objects outside but near the light bundles – there can be more images. The observer sees the images in directions corresponding to the tangents to the real incoming light paths.

In Figure 1, the corresponding angles and angular diameter distances D_L, D_S, D_{LS} are indicated. (In cosmology, the various methods to define distance diverge. The relevant distances for gravitational lensing are the angular diameter distances.) In the thin-lens approximation, the hyperbolic paths are approximated by their asymptotes. In the circular-symmetric case, the deflection angle is given as

$$\tilde{\alpha}(\xi) = \frac{4GM(\xi)}{c^2} \frac{1}{\xi} \quad [4]$$

where $M(\xi)$ is the mass inside a radius ξ . In this depiction, the origin is chosen at the observer. From the diagram, it can be seen that the following relation holds:

$$\theta D_S = \beta D_S + \tilde{\alpha} D_{LS} \quad [5]$$

(for $\theta, \beta, \tilde{\alpha} \ll 1$; this condition is fulfilled in practically all astrophysically relevant situations). With the definition of the reduced deflection angle as $\alpha(\theta) = (D_{LS}/D_S)\tilde{\alpha}(\theta)$, this can be expressed as

$$\beta = \theta - \alpha(\theta) \quad [6]$$

This relation between the positions of images and source can easily be derived for a nonsymmetric mass distribution as well. In that case, all angles are

vector valued. The two-dimensional lens equation then reads

$$\beta = \theta - \alpha(\theta) \quad [7]$$

Einstein Radius

For a point lens of mass M , the deflection angle is given by eqn [4]. Plugging this deflection angle into eqn [6] and using the relation $\xi = D_L \theta$ (cf. Figure 1), one obtains

$$\beta(\theta) = \theta - \frac{D_{LS}}{D_L D_S} \frac{4GM}{c^2 \theta} \quad [8]$$

For the special case in which the source lies exactly behind the lens ($\beta=0$), due to the symmetry, a ring-like image occurs whose angular radius is called Einstein radius θ_E :

$$\theta_E = \sqrt{\frac{4GM}{c^2} \frac{D_{LS}}{D_L D_S}} \quad [9]$$

The Einstein radius defines the angular scale for a lens situation. For a massive galaxy with a mass of $M = 10^{12} M_\odot$ at a redshift of $z_L = 0.5$ and a source at redshift $z_S = 2.0$ (we used here $H = 50 \text{ km s}^{-1} \text{ Mpc}^{-1}$ as the value of the Hubble constant and an Einstein-de Sitter universe), the Einstein radius is

$$\theta_E \approx 1.8 \sqrt{\frac{M}{10^{12} M_\odot}} \text{ arcsec} \quad [10]$$

(note that for cosmological distances, in general, $D_{LS} \neq D_S - D_L$!). For a galactic microlensing scenario in which stars in the disk of the Milky Way act as lenses for stars close to its center, the scale defined by the Einstein radius is

$$\theta_E \approx 0.5 \sqrt{\frac{M}{M_\odot}} \text{ marcsec} \quad [11]$$

An application and some illustrations of the point lens case can be found in the section on galactic microlensing.

Critical Surface Mass Density

In the more general case of a three-dimensional mass distribution of an extended lens, the density $\rho(\mathbf{r})$ can be projected along the line of sight onto the lens plane to obtain the two-dimensional surface mass density distribution $\Sigma(\xi)$ as

$$\Sigma(\xi) = \int_0^{D_S} \rho(\mathbf{r}) dz \quad [12]$$

Here \mathbf{r} is a three-dimensional vector in space, and ξ is a two-dimensional vector in the lens plane. The

two-dimensional deflection angle $\tilde{\alpha}$ is then given as the sum over all mass elements in the lens plane:

$$\tilde{\alpha}(\xi) = \frac{4G}{c^2} \int \frac{(\xi - \xi') \Sigma(\xi')}{|\xi - \xi'|^2} d^2 \xi' \quad [13]$$

For a finite circle with constant surface mass density Σ , the deflection angle can be written as

$$\alpha(\xi) = \frac{D_{LS}}{D_S} \frac{4G \Sigma \pi \xi^2}{c^2 \xi} \quad [14]$$

With $\xi = D_L \theta$ this simplifies to

$$\alpha(\theta) = \frac{4\pi G \Sigma D_L D_{LS}}{c^2} \theta \quad [15]$$

With the definition of the critical surface mass density Σ_{crit} as

$$\Sigma_{\text{crit}} = \frac{c^2}{4\pi G} \frac{D_S}{D_L D_{LS}} \quad [16]$$

the deflection angle for a such a mass distribution can be expressed as

$$\tilde{\alpha}(\theta) = \frac{\Sigma}{\Sigma_{\text{crit}}} \theta \quad [17]$$

The critical surface mass density can be visualized as the lens mass M “smeared out” over the area of the Einstein ring: $\Sigma_{\text{crit}} = M / (R_E^2 \pi)$, where $R_E = \theta_E D_L$. The value of the critical surface mass density is roughly $\Sigma_{\text{crit}} \approx 0.8 \text{ g cm}^{-2}$ for lens and source redshifts of $z_L = 0.5$ and $z_S = 2.0$, respectively. For an arbitrary mass distribution, the condition $\Sigma > \Sigma_{\text{crit}}$ at any point is sufficient to produce multiple images.

Image Positions and Magnifications

The lens equation [6] can be re-formulated in the case of a single-point lens:

$$\beta = \theta - \frac{\theta_E^2}{\theta} \quad [18]$$

Solving this for the image positions θ , one finds that an isolated point source always produces two images of a background source. The positions of the images are given by the two solutions:

$$\theta_{1,2} = \frac{1}{2} \left(\beta \pm \sqrt{\beta^2 + 4\theta_E^2} \right) \quad [19]$$

The magnification of an image is defined by the ratio between the solid angles of the image and the source, since the surface brightness is conserved. Hence, the magnification μ is given as

$$\mu = \frac{\theta d\theta}{\beta d\beta} \quad [20]$$

In the symmetric case above, the image magnification can be written as (by using the lens equation)

$$\mu_{1,2} = \left(1 - \left[\frac{\theta_E}{\theta_{1,2}}\right]^4\right)^{-1} = \frac{u^2 + 2}{2u\sqrt{u^2 + 4}} \pm \frac{1}{2} \quad [21]$$

Here we defined u as the “impact parameter,” the angular separation between lens and source in units of the Einstein radius: $u = \beta/\theta_E$. The magnification of one image (the one inside the Einstein radius) is negative. This means it has negative parity: it is mirror-inverted. For $\beta \rightarrow 0$ the magnification diverges. In the limit of geometrical optics, the Einstein ring of a point source has infinite magnification! (Due to the fact that physical objects have a finite size, and also because at some limit wave optics has to be applied, in reality the magnification stays finite.) The sum of the absolute values of the two image magnifications is the measurable total magnification μ :

$$\mu = |\mu_1| + |\mu_2| = \frac{u^2 + 2}{u\sqrt{u^2 + 4}} \quad [22]$$

Note that this value is (always) larger than 1! (This does not violate energy conservation, since this is the magnification relative to an “empty” universe and not relative to a “smoothed out” universe. This issue is treated in detail in Schneider *et al.* (1992, chapter 4.5).) The “sum” of the two image magnifications is unity:

$$\mu_1 + \mu_2 = 1 \quad [23]$$

(Non)Singular Isothermal Sphere

A popular model for galaxy lenses is the singular isothermal sphere with a three-dimensional density distribution of

$$\rho(r) = \frac{\sigma_v^2}{2\pi G} \frac{1}{r^2} \quad [24]$$

where σ_v is the one-dimensional velocity dispersion. Projecting the matter on a plane, one obtains the circularly symmetric surface mass distribution

$$\Sigma(\xi) = \frac{\sigma_v^2}{2G} \frac{1}{\xi} \quad [25]$$

With $M(\xi) = \int_0^\xi \Sigma(\xi') 2\pi \xi' d\xi'$ plugged into eqn [4], one obtains the deflection angle for an isothermal sphere, which is a constant (i.e., independent of the impact parameter ξ):

$$\tilde{\alpha}(\xi) = 4\pi \frac{\sigma_v^2}{c^2} \quad [26]$$

In practical units for the velocity dispersion of a galaxy, this can be expressed as

$$\tilde{\alpha}(\xi) = 1.15 \left(\frac{\sigma_v}{200 \text{ km s}^{-1}} \right)^2 \text{ arcsec} \quad [27]$$

Two generalizations of this isothermal model are commonly used: models with finite cores are more realistic for (spiral) galaxies. In this case, the deflection angle is modified to (core radius ξ_c):

$$\tilde{\alpha}(\xi) = 4\pi \frac{\sigma_v^2}{c^2} \frac{\xi}{(\xi_c^2 + \xi^2)^{1/2}} \quad [28]$$

Furthermore, a realistic galaxy lens usually is not perfectly symmetric but is slightly elliptical. Depending on whether one wants an elliptical mass distribution or an elliptical potential, various formalisms are in use.

Lens Mapping

In the vicinity of an arbitrary point, the lens mapping as shown in eqn [7] can be described by its Jacobian matrix \mathcal{A} :

$$\mathcal{A} = \frac{\partial \boldsymbol{\beta}}{\partial \boldsymbol{\theta}} = \left(\delta_{ij} - \frac{\partial \alpha_i(\boldsymbol{\theta})}{\partial \theta_j} \right) = \left(\delta_{ij} - \frac{\partial^2 \psi(\boldsymbol{\theta})}{\partial \theta_i \partial \theta_j} \right) \quad [29]$$

Here we made use of the fact that the deflection angle can be expressed as the gradient of an effective two-dimensional scalar potential ψ : $\nabla_\theta \psi = \boldsymbol{\alpha}$, where

$$\psi(\boldsymbol{\theta}) = \frac{D_{LS}}{D_L D_S} \frac{2}{c^2} \int \Phi(\mathbf{r}) d\mathbf{z} \quad [30]$$

and $\Phi(\mathbf{r})$ is the Newtonian potential of the lens. The determinant of the Jacobian \mathcal{A} is the inverse of the magnification:

$$\mu = \frac{1}{\det \mathcal{A}} \quad [31]$$

Defining

$$\psi_{ij} = \frac{\partial^2 \psi}{\partial \theta_i \partial \theta_j} \quad [32]$$

the Laplacian of the effective potential ψ is twice the convergence:

$$\psi_{11} + \psi_{22} = 2\kappa = \text{tr } \psi_{ij} \quad [33]$$

With the definitions of the components of the external shear γ ,

$$\gamma_1(\boldsymbol{\theta}) = \frac{1}{2}(\psi_{11} - \psi_{22}) = \gamma(\boldsymbol{\theta}) \cos[2\varphi(\boldsymbol{\theta})] \quad [34]$$

and

$$\gamma_2(\boldsymbol{\theta}) = \psi_{12} = \psi_{21} = \gamma(\boldsymbol{\theta}) \sin[2\varphi(\boldsymbol{\theta})] \quad [35]$$

(where the angle φ reflects the direction of the shear-inducing tidal force relative to the coordinate system), the Jacobian matrix can be written as

$$\mathcal{A} = \begin{pmatrix} 1 - \kappa - \gamma_1 & -\gamma_2 \\ -\gamma_2 & 1 - \kappa + \gamma_1 \end{pmatrix} \\ = (1 - \kappa) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \gamma \begin{pmatrix} \cos 2\varphi & \sin 2\varphi \\ \sin 2\varphi & -\cos 2\varphi \end{pmatrix} \quad [36]$$

The magnification can now be expressed as a function of the local convergence κ and the local shear γ :

$$\mu = (\det \mathcal{A})^{-1} = \frac{1}{(1 - \kappa)^2 - \gamma^2} \quad [37]$$

Locations at which $\det \mathcal{A} = 0$ have formally infinite magnification. They are called “critical curves” in the lens plane. The corresponding locations in the source plane are the “caustics.” For spherically symmetric mass distributions, the critical curves are circles. For a point lens, the caustic degenerates into a point. For elliptical lenses or spherically symmetric lenses plus external shear, the caustics consist of cusps and folds.

Time Delay and Fermat's Theorem

The deflection angle is the gradient of an effective lensing potential ψ . Hence, the lens equation can be rewritten as

$$(\boldsymbol{\theta} - \boldsymbol{\beta}) - \nabla_{\boldsymbol{\theta}} \psi = 0 \quad [38]$$

or

$$\nabla_{\boldsymbol{\theta}} \left(\frac{1}{2} (\boldsymbol{\theta} - \boldsymbol{\beta})^2 - \psi \right) = 0 \quad [39]$$

The term in brackets appears as well in the physical time delay function for gravitationally lensed images:

$$\tau(\boldsymbol{\theta}, \boldsymbol{\beta}) = \tau_{\text{geom}} + \tau_{\text{grav}} \\ = \frac{1 + z_L}{c} \frac{D_L D_S}{D_{LS}} \left(\frac{1}{2} (\boldsymbol{\theta} - \boldsymbol{\beta})^2 - \psi(\boldsymbol{\theta}) \right) \quad [40]$$

This time delay surface is a function of the image geometry $(\boldsymbol{\theta}, \boldsymbol{\beta})$, the gravitational potential ψ , and the distances D_L , D_S , and D_{LS} . The first part – the geometrical time delay τ_{geom} – reflects the extra path length compared to the direct line between observer and source. The second part – the gravitational time delay τ_{grav} – is the retardation due to gravitational potential of the lensing mass (known and confirmed as Shapiro delay in the solar system). From eqns [39] and [40], it follows that the gravitationally lensed images appear at locations that correspond to

extrema in the light travel time, which reflects Fermat's principle in gravitational-lensing optics.

The (angular-diameter) distances that appear in eqn [40] depend on the value of the Hubble constant. Therefore, it is possible to determine the latter by measuring the time delay between different images and using a good model for the effective gravitational potential ψ of the lens.

Lensing Phenomena

Strong lensing phenomena involve multiple images, caustics, critical lines, usually a significant magnification, and large distortions if extended sources are involved. Below we discuss the most frequent strong lensing phenomena.

Galactic Microlensing

The conceptually simplest strong lensing scenario is a foreground star acting as a lens on a background star. Since stars in the Milky Way move relative to each other, this can be observed as a time-variable situation: due to the relative motion between observer, lensing star, and source star, the projected impact parameter between lens and source changes with time and produces a time-dependent magnification. If the impact parameter is smaller than an Einstein radius ($u < 1$), then the magnification is $\mu_{\text{min}} > 1.34$ (cf. eqn [22]).

For an extended source, a sequence image configurations with decreasing impact parameter is illustrated in Figure 2 for five instants of time. The separation of the two images is of order-2 Einstein radii when they are of comparable magnification, which corresponds to only about 1 marcsec in a realistic situation in the Milky Way. Hence, the two images cannot be resolved individually; we can only observe the combined brightness of the image pair. This is illustrated in Figures 3 and 4, which show the relative tracks and the respective light curves for five values of the minimum impact parameter u_{min} .

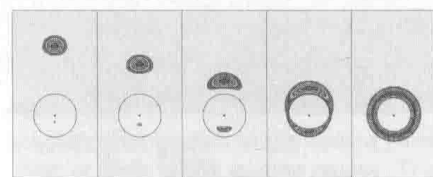


Figure 2 Five snapshots of a gravitational lens situation with a point lens and an extended source: from left to right the alignment between lens and source gets better and better, until it is perfect in the rightmost panel. This results in the image of an “Einstein ring.”

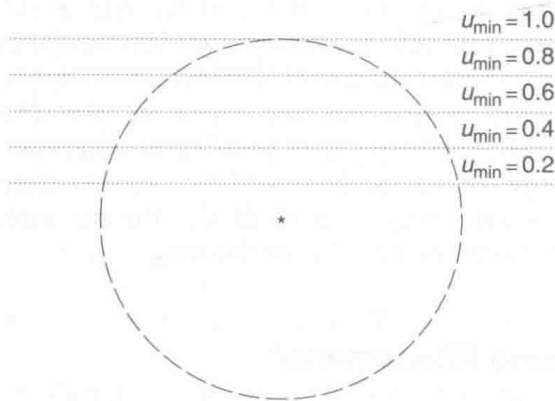


Figure 3 Five relative tracks between background star and foreground lens (indicated as the central star) parametrized by the impact parameter u_{\min} . The dashed line indicates the Einstein ring for the lens.

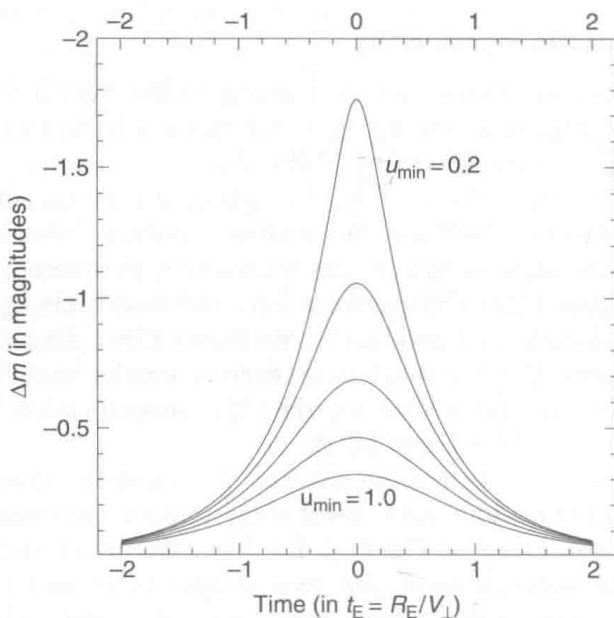


Figure 4 Five microlensing light curves for the tracks indicated in **Figure 3**, parametrized by the impact parameter u_{\min} . The vertical axis is the magnification in astronomical magnitudes relative to the unlensed case, the horizontal axis displays the time in “normalized” units.

Quantitatively, the total magnification $\mu = |\mu_1| + |\mu_2|$ of the two images (cf. eqn [22]) entirely depends on the impact parameter $u(t) = r(t)/R_E$ between the lensed star and the lensing object, measured in the lens plane (here R_E is the Einstein radius of the lens, i.e., the radius at which a circular image appears for perfect alignment between source, lens, and observer, cf. **Figure 2**, rightmost panel):

$$\mu(u(t)) = \frac{u(t)^2 + 2}{u(t)\sqrt{u(t)^2 + 4}} \quad [41]$$

The timescale of such a “microlensing event” is defined as the time it takes for the source to cross

the Einstein radius. With realistic values for distances and relative velocity, this can be expressed as

$$t_0 = \frac{R_E}{v_{\perp}} \approx (0.214 \text{ yr}) \sqrt{\frac{M}{M_{\odot}}} \sqrt{\frac{D_L}{10 \text{ kpc}}} \times \sqrt{1 - \frac{D_L}{D_S} \left(\frac{v_{\perp}}{200 \text{ km s}^{-1}} \right)^{-1}} \quad [42]$$

(here v_{\perp} is the (relative) transverse velocity of the lens; we applied the simple relation $D_{LS} = D_S - D_L$, which is valid here).

Note that from eqn [42] it is obvious that it is not possible to determine the mass of the lens from one individual microlensing event. The duration of an event is determined by three unknown parameters: the mass of the lens m , the transverse velocity v_{\perp} , and the distance of the lens D_L (assuming we know the distance to the source). It is impossible to disentangle these for individual events. Only with a model for the spatial and velocity distribution of the lensing stars in the Milky Way, one can obtain approximate information about the masses of the lensing objects.

In 1986, Bohdan Paczyński suggested to use this microlensing method as an observational test for potential dark matter candidates in the halo of the Milky Way. If the dark matter is in the form of astrophysical objects (such as brown dwarfs, neutron stars, black holes, sometimes called “MACHO” for MAssive Compact Halo Object), then they should occasionally act as lenses on stars in the neighboring galaxy Large Magellanic Cloud. It turned out that too few of such microlensing events were observed, in order to explain the dark matter this way.

However, this method produced more than 2000 microlensing events by ordinary stars in the direction to the center of the Milky Way. Two of these events provide convincing evidence for a planet accompanying the lensing star. It is likely that gravitational microlensing will provide a statistically very valuable sample of extrasolar planets, because in contrast to most other methods these planets are pre-selected by their host stars. Furthermore, microlensing is sensitive to masses as low as a few Earth masses.

Multiply-Imaged Quasars

The first gravitationally lensed double quasar was discovered in 1979: two images of the same quasar, separated by about 6 arcsec. This led to the field of gravitational lensing as an observational science. By now, more than 120 multiply imaged quasars are known, mostly double and quadruple images. They

span image separations from 0.3 arcsec to almost 30 arcsec.

Gravitationally lensed quasar systems are studied individually in great detail to get a better understanding of both lens and source. The lens systems are analyzed statistically as well, in order to get information about the population of lenses (and quasars) in the universe, their distribution in distance (i.e., cosmic time) and mass, and hence about the cosmological model.

Time delay and Hubble constant As stated above, the signals from a gravitational lens system reach us with a certain “time delay” Δt , so that the measured fluxes as functions of time, $I_A(t)$ and $I_B(t)$, can be described as: $I_B(t) = \text{const.} \times I_A(t + \Delta t)$. Any intrinsic fluctuation of the quasar shows up in both images, in general with an overall offset in apparent magnitude and an offset in time.

Q0957 + 561 is the first lens system in which the time delay was firmly established:

$$\Delta t_{\text{Q0957+561}} = (417 \pm 3) \text{ days} \quad [43]$$

With a model of the lens system, the time delay can be used to determine the Hubble constant. (This can be seen very simply: imagine a certain lens situation like the one displayed in Figure 1. If now all length scales are reduced by a factor of 2 and at the same time all masses are reduced by a factor of 2, then for an observer, the angular configuration in the sky would appear exactly identical. But the total length of the light path is reduced by a factor of 2. Now, since the time delay between the two paths is the same fraction of the total lengths in either scenario, a measurement of this fractional length allows us to determine the total length, and hence the Hubble constant, the constant of proportionality between distance and redshift.) The resulting value of H_0 is

$$H_0 = (67 \pm 13) \text{ km s}^{-1} \text{ Mpc}^{-1} \quad [44]$$

where the uncertainty comprises the 95% confidence level. To date, about a dozen quasar lens systems have measured time delays. The derived values of the Hubble constant are “lowish,” if we assume the best astrophysical motivated lens models.

Quasar Microlensing

Light bundles from “lensed” quasars are split by intervening galaxies. Usually the quasar light bundle passes through the galaxy and/or the galaxy halo. Galaxies consist at least partly of stars, and galaxy halos consist possibly of compact objects as well.

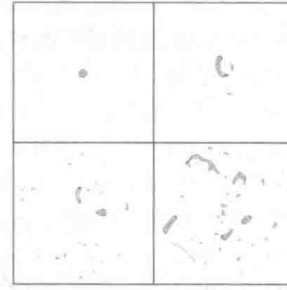


Figure 5 “Microimages”: the top left panel shows an assumed “unlensed” source profile of a quasar. The other three panels illustrate the microimage configuration as it would be produced by stellar objects in the foreground. The surface mass density of the lenses is 20% (top right), 50% (bottom left), and 80% (bottom right) of the critical density (cf. eqn [16]).

Each of these stars (or other compact objects like black holes, brown dwarfs, or planets) acts as a “compact lens” or “microlens” and produces at least one additional microimage of the source. This means the “macroimage” consists of many “microimages” (Figure 5). But because the image splitting is proportional to the square root of the lens mass, these microimages are only of order a microarcsecond apart and cannot be resolved. Various aspects of microlensing have been addressed after the first double quasar had been discovered.

The microlenses produce a complicated two-dimensional magnification distribution in the source plane. It consists of many caustics, locations that correspond to formally infinitely high magnification. An example for such a magnification pattern is shown in Figure 6. It is determined with the parameters of image A of the quadruple quasar Q2237 + 0305

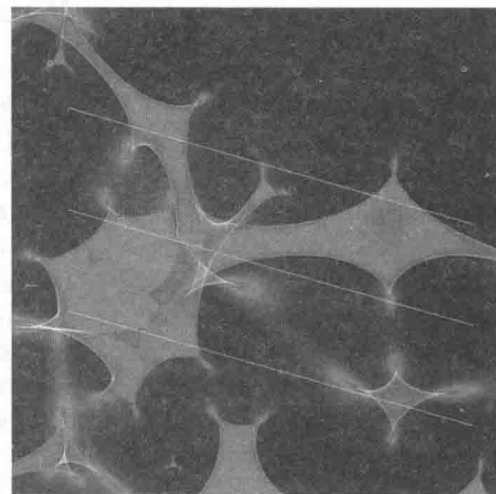


Figure 6 Magnification pattern in the source plane, produced by a dense field of stars in the lensing galaxy. The gray scale reflects the magnification as a function of the quasar position. Light curves taken along the straight tracks are shown in Figure 7. The microlensing parameters were chosen according to a model for image A of the quadruple quasar Q2237 + 0305: $\kappa = 0.36$, $\gamma = 0.44$.

(surface mass density $\kappa=0.36$; external shear $\gamma=0.44$). Gray scale indicates the magnification.

Due to the relative motion between observer, lens, and source, the quasar changes its position relative to this arrangement of caustics, that is, the apparent brightness of the quasar changes with time. A one-dimensional cut through such a magnification pattern, convolved with a source profile of the quasar, results in a microlensed light curve. Examples for microlensed light curves taken along the straight lines in Figure 6 can be seen in Figure 7 for two different quasar sizes.

In particular when the quasar track crosses a caustic (the sharp lines in Figure 6 for which the magnification formally is infinite, because the determinant of the Jacobian disappears, cf. eqn [31]), a pair of highly magnified microimages appears newly or merges and disappears. Such a microlensing event can easily be detected as a strong peak in the light curve of the quasar image.

Microlens-induced fluctuations in the observed brightness of quasars contain information both about the light-emitting source (size of continuum region or broad line region of the quasar, brightness profile of quasar) and about the lensing objects (masses, density, transverse velocity). Hence, from a comparison between observed and simulated quasar microlensing, one can draw conclusions about the density and mass scale of the microlenses. So far the "best" example of a microlensed quasar is the quadruple quasar Q2237 + 0305.

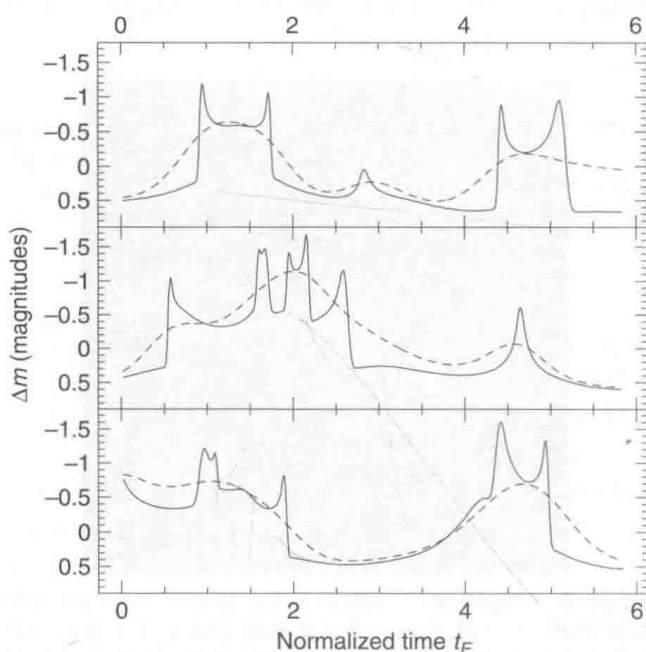


Figure 7 Microlensing light curve for the straight lines in Figure 6. The solid and dashed lines indicate relatively small and large quasar sizes. The time axis is in units of Einstein radii divided by unit velocity.

Einstein Rings

If a point source lies exactly behind a point lens, a ring-like image occurs. Theorists had recognized early on that such a symmetric lensing arrangement would result in a ring image, the so-called "Einstein ring." There are two necessary requirements for the observability of Einstein rings: the mass distribution of the lens needs to be approximately axially symmetric, as seen from the observer, and the source must lie exactly on top of the resulting degenerate pointlike caustic. Such a geometric arrangement is highly unlikely for pointlike sources. But astrophysical sources in the real universe have a finite extent, and it is enough if a part of the source covers the point caustic (or the complete astroid caustic in the case of a not quite axially symmetric mass distribution) in order to produce such an annular image.

In 1988, the first example of an "Einstein ring" was discovered. With high-resolution radio observations, the extended radio source MG1131 + 0456 turned out to be a ring with a diameter of about 1.75 arcsec. The source was identified as a radio lobe at a redshift of $z_s=1.13$, whereas the lens is a galaxy at $z_L=0.85$. By now more than a dozen cases have been found that qualify as Einstein rings. Their diameters vary between 0.33 and about 2 arcsec.

Giant Luminous Arcs and Arclets

Fritz Zwicky had pointed out the potential use of galaxies and galaxy clusters as gravitational lenses in the 1930s. With background galaxies as sources, the apparent lensing consequences for them would be far more dramatic than for quasars: galaxies should be heavily deformed once they are strongly lensed. Rich clusters of galaxies at redshifts beyond $z \approx 0.2$ with masses of order $10^{14} M_\odot$ are very effective lenses if they are centrally concentrated. Their Einstein radii are of the order of 20 arcsec.

In 1986, the following gravitational lensing phenomenon was discovered: magnified, distorted, and strongly elongated images of background galaxies which happen to lie behind foreground clusters of galaxies, the so-called giant luminous arcs. The giant arcs can be exploited in two ways, as is typical for many lens phenomena. Firstly, they provide us with strongly magnified galaxies at (very) high redshifts. These galaxies would be too faint to be detected or analyzed in their unlensed state. Hence, with the lensing boost, we can study these galaxies in their early evolutionary stages, possibly as infant or protogalaxies, relatively shortly after the big bang. The other practical application of the arcs is to take them as tools to study the potential and mass distribution of the lensing galaxy cluster. In the simplest model of a spherically symmetric mass distribution for the cluster,

giant arcs form very close to the critical curve, which marks the Einstein ring. So with the redshifts of the cluster and the arc, it is easy to determine a rough estimate of the lensing mass by just determining the radius of curvature and interpreting it as the Einstein radius of the lens system.

Weak Lensing/Statistical Lensing/Cosmic Shear

In contrast to the phenomena that were mentioned here, “weak lensing” deals with effects of light deflection that cannot be measured individually, but rather in a statistical way only. No caustics, critical lines, or multiple images are involved. As was discussed above, “strong lensing” – usually defined as the regime that involves multiple images, high magnifications, and caustics in the source plane – is a rare phenomenon. Weak lensing on the other hand is much more common. In principle, weak lensing acts along each line of sight in the universe, since each light bundle’s path is affected by matter inhomogeneities along or near its path. It is just a matter of how accurately we can measure. In recent years, many teams started impressive and ambitious observational programs to determine the slight distortion of tens of thousands of background galaxies by foreground galaxy clusters and/or by the large-scale structure in the universe, the so-called cosmic shear. It is beyond the scope of this article to discuss these applications of weak gravitational lensing. The interested reader is referred to the “Further reading” section, in particular to Bartelmann and Schneider (2001).

See also: Cosmology: Mathematical Aspects; General Relativity: Experimental Tests; General Relativity: Overview; Newtonian Limit of General Relativity; Singularity and Bifurcation Theory.

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Gravitational N-Body Problem (Classical)

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Introduction

Let a number, N , of particles interact classically through Newton's laws of motion and Newton's inverse-square law of gravitation. Then the equations of motion are

$$\ddot{\mathbf{r}}_i = -G \sum_{j=1, j \neq i}^N m_j \frac{\mathbf{r}_i - \mathbf{r}_j}{|\mathbf{r}_i - \mathbf{r}_j|^3} \quad [1]$$

where \mathbf{r}_i is the position vector of the i th particle relative to some inertial frame, G is the universal constant of gravitation, and m_i is the mass of the i th particle. These equations provide an approximate

mathematical model with numerous applications in astrophysics, including the motion of the Moon and other bodies in the solar system (planets, asteroids, comets, and meteor particles); stars in stellar systems ranging from binary and other multiple stars to star clusters and galaxies; and the motion of dark-matter particles in cosmology. For $N=1$ and $N=2$, the equations can be solved analytically. The case $N=3$ provides one of the richest of all unsolved dynamical problems – the general three-body problem. For problems dominated by one massive body, as in many planetary problems, approximate methods based on perturbation expansions have been developed. In stellar dynamics, astrophysicists have developed numerous numerical and theoretical approaches to the problem for larger values of N , including treatments based on the Boltzmann equation and the Fokker–Planck equation; such N -body systems can also be modeled as self-gravitating

gases, and thermodynamic insights underpin much of our qualitative understanding.

Few-Body Problems

The Two-Body Problem

For $N=2$, the relative motion of the two bodies can be reduced to the force-free motion of the center of mass and the problem of the relative motion. If $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$, then

$$\ddot{\mathbf{r}} = -G(m_1 + m_2) \frac{\mathbf{r}}{|\mathbf{r}|^3} \quad [2]$$

often called the Kepler problem. It represents motion of a particle of unit mass under a central inverse-square force of attraction. Energy and angular momentum are constant, and the motion takes place in a plane passing through the origin. Using plane polar coordinates (r, θ) in this plane, the equations for the energy and angular momentum reduce to

$$E = \frac{1}{2} \left(\dot{r}^2 + \frac{L^2}{r^2} \right) - \frac{G(m_1 + m_2)}{r} \quad [3]$$

$$L = r^2 \dot{\theta} \quad [4]$$

(Note that these are not the energy and angular momentum of the two-body problem, even in the barycentric frame of the center of mass; E and L must be multiplied by the reduced mass $m_1 m_2 / (m_1 + m_2)$.) Using eqns [3] and [4], the problem is reduced to quadratures. The solution shows that the motion is on a conic section (ellipse, circle, straight line, parabola, or hyperbola), with the origin at one focus.

This reduction depends on the existence of integrals of the equations of motion, and these in turn depend on symmetries of the underlying Lagrangian or Hamiltonian. Indeed, eqns [1] yield ten first integrals: six yield the rectilinear motion of the center of mass, three the total angular momentum, and one the energy. Furthermore, eqn [2] may be transformed, via the Kustaanheimo–Stiefel (KS) transformation, to a four-dimensional simple harmonic oscillator. This reveals further symmetries, corresponding to further invariants: the three components of the Lenz vector. Another manifestation of the abundance of symmetries of the Kepler problem is the fact that there exist action-angle variables in which the Hamiltonian depends only on one action, that is, $H = H(L)$. Another application of the KS transformation is one that has practical importance: it removes the singularity of (i.e., regularizes) the Kepler problem at $r=0$, which is troublesome numerically.

To illustrate the character of the KS transformation, we consider briefly the planar case, which can

be handled with a complex variable obeying the equation of motion $\ddot{z} = -z/|z|^3$ (after scaling eqn (2)). By introducing the Levi-Civita transformation $z = Z^2$ and Sundman's transformation of the time, that is, $dt/d\tau = |z|$, the equation of motion transforms to $Z'' = hZ/2$, where $h = |\dot{z}|^2/2 - 1/|z|$ is the constant of energy. The KS transformation is a very similar exercise using quaternions.

The Restricted Three-Body Problem

The simplest three-body problem is given by the motion of a test particle in the gravitational field of two particles, of positive mass m_1, m_2 , in circular Keplerian motion. This is called the circular restricted three-body problem, and the two massive particles are referred to as primaries. In a rotating frame of reference, with origin at the center of mass of these two particles, which are at rest at positions $\mathbf{r}_1, \mathbf{r}_2$, the equation of motion is

$$\ddot{\mathbf{r}} + 2\boldsymbol{\Omega} \times \dot{\mathbf{r}} + \boldsymbol{\Omega} \times (\boldsymbol{\Omega} \times \mathbf{r}) = G\nabla \left(\frac{m_1}{|\mathbf{r} - \mathbf{r}_1|} + \frac{m_2}{|\mathbf{r} - \mathbf{r}_2|} \right) \quad [5]$$

where \mathbf{r} is the position of the massless particle and $\boldsymbol{\Omega}$ is the angular velocity of the frame.

This problem has three degrees of freedom but only one known integral: it is the Hamiltonian in the rotating frame, and equivalent to the Jacobi integral, J . One consequence is that Liouville's theorem is not applicable, and more elaborate arguments are required to decide its integrability. Certainly, no general analytical solution is known.

There are five equilibrium solutions, discovered by Euler and Lagrange (see Figure 1). They lie at critical points of the effective potential in the

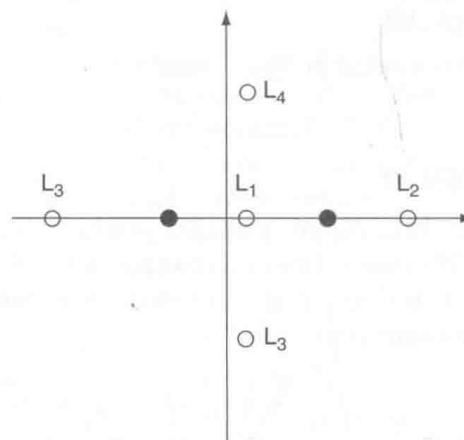


Figure 1 The equilibrium solutions of the circular restricted three-body problem. A rotating frame of reference is chosen in which two particles are at rest on the x -axis. The massless particle is at equilibrium at each of the five points shown. Five similar configurations exist for the general three-body problem; these are the “central” configurations.

rotating frame, and demarcate possible regions of motion.

Throughout the twentieth century, much numerical effort was used in finding and classifying periodic orbits, and in determining their stability and bifurcations. For example, there are families of periodic orbits close to each primary; these are perturbed Kepler orbits, and are referred to as satellite motions. Other important families are the series of Liapounov orbits starting at the equilibrium points.

Some variants of the restricted three-body problem include the following:

1. The elliptic restricted three-body problem, in which the primaries move on an elliptic Keplerian orbit; in suitable coordinates the equation of motion closely resembles eqn [5], except for a factor on the right side which depends explicitly on the independent variable (transformed time); this system has no first integral.
2. Sitnikov's problem, which is a special case of the elliptic problem, in which $m_1 = m_2$, and the motion of the massless particle is confined to the axis of symmetry of the Keplerian motion; this is still nonintegrable, but simple enough to allow extensive analysis of such fundamental issues as integrability and stochasticity.
3. Hill's problem, which is a scaled version suitable for examining motions close to one primary; its importance in applications began with studies of the motion of the moon, and it remains vital for understanding the motion of asteroids.

The General Three-Body Problem

Exact solutions When all three particles have nonzero masses, the equations of motion become

$$m_i \ddot{\mathbf{r}}_i = -\nabla_i W$$

where the potential energy is

$$W = -G \sum_{1 \leq i < j \leq 3} \frac{m_i m_j}{|\mathbf{r}_i - \mathbf{r}_j|}$$

Then the exact solutions of Euler and Lagrange survive in the form of homographic solutions. In these solutions, the configuration remains geometrically similar, but may rotate and/or pulsate in the same way as in the two-body problem.

Let us represent the position vector \mathbf{r}_i in the planar three-body problem by the complex number z_i . Then, it is easy to see that we have a solution of the form $z_i(t) = z(t)z_{0i}$, provided that

$$\ddot{z} = -C \frac{z}{|z|^3}$$

and

$$m_i C z_{0i} = \nabla_i W(z_{01}, z_{02}, z_{03})$$

for some constant C . Thus, $z(t)$ may take the form of any solution of the Kepler problem, while the complex numbers z_{0i} must correspond to what is called a central configuration. These are in fact critical points of the scale-free function $W\sqrt{I}$, where I (the "moment of inertia of the system") is given by $I = \sum_1^3 m_i r_i^2$; and $C = -W/I$.

The existence of other important classes of periodic solutions can be proved analytically, even though it is not possible to express the solution in closed form. Examples include hierarchical three-body systems, in which two masses m_1, m_2 exhibit nearly elliptic relative motion, while a third mass orbits the barycenter of m_1 and m_2 in another nearly elliptic orbit. In the mathematical literature, this is referred to as motion of elliptic-elliptic type. More surprisingly, the existence of a periodic solution in which the three bodies travel in succession along the same path, shaped like a figure 8 (cf. Figure 2), was established by Chenciner and Montgomery (2000), following its independent discovery by Moore using numerical methods. Another interesting periodic motion that was discovered numerically, by Schubart, is a solution of the collinear three-body problem, and so collisions are inevitable. In this motion, the body in the middle alternately encounters the other two bodies.

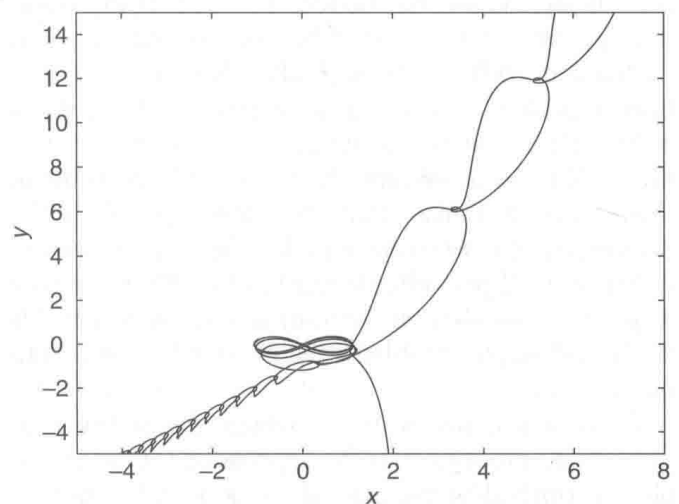


Figure 2 A rare example of a scattering encounter between two binaries (which approach from upper right and lower left) which leads to a permanently bound triple system describing the "figure-8" periodic orbit. A fourth body escapes at the bottom. Note the differing scales on the two axes. (Reproduced with permission from Heggie DC (2000) A new outcome of binary-binary scattering. *Monthly Notices of the Royal Astronomical Society* 318(4): L61–L63; © Blackwell Publishing Ltd.)

Singularities As Schubart's solution illustrates, two-body encounters can occur in the three-body problem. Such singularities can be regularized just as in the pure two-body problem. Triple collisions cannot be regularized in general, and this singularity has been studied by the technique of "blowup." This has been worked out most thoroughly in the collinear three-body problem, which has only two degrees of freedom. The general idea is to transform to two variables, of which one (denoted by r , say) determines the scale of the system, while the other (s) determines the configuration (e.g., the ratio of separations of the three masses). By scaling the corresponding velocities and the time, one obtains a system of three equations of motion for s and the two velocities which are perfectly regular in the limit $r \rightarrow 0$. In this limit, the energy integral restricts the solutions of the system to a manifold (called the collision manifold). Exactly the same manifold results for zero-energy solutions, which permits a simple visualization. Equilibria on the collision manifold correspond to the Lagrangian collinear solutions in which the system either expands to infinity or contracts to a three-body collision.

Qualitative ideas Reference has already been made to motion of elliptic-elliptic type. In a motion of elliptic-hyperbolic type, there is again an "inner" pair of bodies describing nearly Keplerian motion, while the relative motion of the third body is nearly hyperbolic. In applications, this is referred to as a kind of scattering encounter between a binary and a third body. When the encounter is sufficiently close, it is possible for one member of the binary to be exchanged with the third body. One of the major historical themes of the general three-body problem is the classification of connections between these different types of asymptotic motion. It is possible to show, for instance, that the measure of initial conditions of hyperbolic-elliptic type leading asymptotically to elliptic-elliptic motion (or any other type of permanently bound motion) is zero. Much of the study of such problems has been carried out numerically.

There are many ways in which the stability of three-body motions may be approached. One example is furnished by the central configurations already referred to. They can be used to establish sufficient conditions for ensuring that exchange is impossible, and similar conclusions.

A powerful tool for qualitative study of three-body motions is Lagrange's identity, which is now thought of as the reduction to three bodies of the virial theorem. Let the size of the system be

characterized by the "moment of inertia" I . Then it is easy to show that

$$\frac{d^2 I}{dt^2} = 4T + 2W$$

where T , W are, respectively, the kinetic and potential energies of the system. Usually, the barycentric frame is adopted. Since $E = T + V$ is constant and $T \geq 0$, it follows that the system is not bounded for all $t > 0$ unless $E < 0$.

Perturbation theory The question of the integrability of the general three-body problem has stimulated much research, including the famous study by Poincaré which established the nonexistence of integrals beyond the ten classical ones. Poincaré's work was an important landmark in the application to the three-body problem of perturbation methods. If one mass dominates, that is, $m_1 \gg m_2$ and $m_1 \gg m_3$, then the motion of m_2 and m_3 relative to m_1 is a mildly perturbed two-body motion, unless m_2 and m_3 are close together. Then it is beneficial to describe the motion of m_2 relative to m_1 by the parameters of Keplerian motion. These would be constant in the absence of m_3 , and vary slowly because of the perturbation by m_3 . This was the idea behind Lagrange's very general method of variation of parameters for solving systems of differential equations. Numerous methods were developed for the iterative solution of the resulting equations. In this way, the solution of such a three-body problem could be represented as a type of trigonometric series in which the arguments are the angle variables describing the two approximate Keplerian motions. These were of immense value in solving problems of celestial mechanics, that is, the study of the motions of planets, their satellites, comets, and asteroids.

A major step forward was the introduction of Hamiltonian methods. A three-body problem of the type considered here has a Hamiltonian of the form

$$H = H_1(L_1) + H_2(L_2) + R$$

where H_i , $i=1, 2$, are the Hamiltonians describing the interaction between m_i and m_1 , and R is the "disturbing function." It depends on all the variables, but is small compared with the H_i . Now perturbation theory reduces to the task of performing canonical transformations which simplify R as much as possible.

Poincaré's major contribution in this area was to show that the series solutions produced by perturbation methods are not, in general, convergent, but

asymptotic. Thus, they were of practical rather than theoretical value. For example, nothing could be proved about the stability of the solar system using perturbation methods. It took the further analytic development of KAM theory to rescue this aspect of perturbation theory. This theory can be used to show that, provided that two of the three masses are sufficiently small, then for almost all initial conditions the motions remain close to Keplerian for all time. Unfortunately, now it is the practical aspect of the theory which is missing; though we have introduced this topic in the context of the three-body problem, it is extensible to any N -body system with $N - 1$ small masses in nearly Keplerian motion about m_1 , but to be applicable to the solar system the masses of the planets would have to be ridiculously small.

Numerical methods Numerical integrations of the three-body problem were first carried out near the beginning of the twentieth century, and are now commonplace. For typical scattering events, or other short-lived solutions, there is usually little need to go beyond common Runge–Kutta methods, provided that automatic step-size control is adopted. When close two-body approaches occur, some regularization based on the KS transformation is often exploited. In cases of prolonged elliptic–elliptic motion, an analytic approximation based on Keplerian motion may be adequate. Otherwise (as in problems of planetary motion, where the evolution takes place on an extremely long timescale), methods of very high order are often used. Symplectic methods, which have been developed in the context of Hamiltonian problems, are increasingly adopted for problems of this kind, as their long-term error behavior is generally much superior to that of methods which ignore the geometrical properties of the equations of motion.

Four- and Five-Body Problems

Many of the foregoing remarks, on central configurations, numerical methods, KAM theory, etc., apply equally to few-body problems with $N > 3$. Of special interest from a theoretical point of view is the occurrence of a new kind of singularity, in which motions become unbounded in finite time. For $N = 4$, the known examples also require two-body collisions, but noncollision orbits exhibiting finite-time blowup are known for $N = 5$.

One of the practical (or, at least, astronomical) applications is again to scattering encounters, this time involving the approach of two binaries on a hyperbolic relative orbit. Numerical results show

that a wide variety of outcomes is possible, including even the creation of the figure-8 periodic orbit of the three-body problem, while a fourth body escapes (Figure 2).

Many-Body Problems

Many of the concepts already introduced, such as the virial theorem, apply equally well to the many-body classical gravitational problem. This section refers mainly to the new features which arise when N is not small. In particular, statistical descriptions become central. The applications also have a different emphasis, moving from problems of planetary dynamics (celestial mechanics) to those of stellar dynamics. Typically, N lies in the range 10^2 – 10^{12} .

Evolution of the Distribution Function

The most useful statistical description is obtained if the correlations we neglect and focus on the one-particle distribution function $f(\mathbf{r}, \mathbf{v}, t)$, which can be interpreted as the number density at time t at the point in phase space corresponding to position \mathbf{r} and velocity \mathbf{v} . Several processes contribute to the evolution of f .

Collective effects When the effects of near neighbors are neglected, the dynamics is described by the Vlasov–Poisson system

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} - \frac{\partial \phi(\mathbf{r}, t)}{\partial \mathbf{r}} \cdot \frac{\partial f}{\partial \mathbf{v}} = 0 \quad [6]$$

$$\nabla^2 \phi = 4\pi G m \int f(\mathbf{r}, \mathbf{v}, t) d^3 \mathbf{v} \quad [7]$$

where ϕ is the gravitational potential and m is the mass of each body. Obvious extensions are necessary if not all bodies have the same mass.

Solutions of eqn [6] may be found by the method of characteristics, which is most useful in cases where the equation of motion $\ddot{\mathbf{r}} = -\nabla \phi$ is integrable, for example, in stationary, spherical potentials. An example is the solution

$$f = |E|^{7/2} \quad [8]$$

where E is the specific energy of a body, that is, $E = v^2/2 + \phi$. This satisfies eqn [6] provided that ϕ is static. Equation [7] is satisfied provided that ϕ satisfies a case of the Lane–Emden equation, which is easy to solve in this case.

The solution just referred to is an example of an equilibrium solution. In an equilibrium solution, the virial theorem takes the form $4T + 2W = 0$, where

T , W are appropriate mean-field approximations for the kinetic and potential energy, respectively. It follows that $E = -T$, where $E = T + V$ is the total energy. An increase in E causes a decrease in T , which implies that a self-gravitating N -body system exhibits a negative specific heat.

There is little to choose between one equilibrium solution and another, except for their stability. In such an equilibrium, the bodies orbit within the potential on a timescale of the crossing time, which is conventionally defined to be

$$t_{\text{cr}} = \frac{GM^{5/2}}{(2|E|)^{3/2}}$$

The most important evolutionary phenomenon of collisionless dynamics is violent relaxation. If f is not time independent then ϕ is time dependent in general. Also, from the equation of motion of one body, E varies according to $dE/dt = \partial\phi/\partial t$, and so energy is exchanged between bodies, which leads to an evolution of the distribution of energies. This process is known as violent relaxation.

Two other relaxation processes are of importance:

1. Relaxation is possible on each energy hypersurface, even in a static potential, if the potential is nonintegrable.
2. The range of collective phenomena becomes remarkably rich if the system exhibits ordered motions, as in rotating systems. Then an important role is played by resonant motions, especially resonances of low order. The corresponding theory lies at the basis of the theory of spiral structure in galaxies, for instance.

Collisional effects The approximations of collisionless stellar dynamics suppress two important processes:

1. The exponential divergence of stellar orbits, which takes place on a timescale of order t_{cr} . Even in an integrable potential, therefore, f evolves on each energy hypersurface.
2. Two-body relaxation. It operates on a timescale of order $(N/\ln N)t_{\text{cr}}$, where N is the number of particles. Although this two-body relaxation timescale, t_r , is much longer than any other timescale we have considered, this process leads to evolution of $f(E)$, and it dominates the long-term evolution of large N -body systems. It is usually modeled by adding a collision term of Fokker-Planck type on the right-hand side of eqn [6].

In this case, the only equilibrium solutions in a steady potential are those in which $f(E) \propto \exp(-\beta E)$, where β is a constant. Then eqn [7]

becomes Liouville's equation, and for the case of spherical symmetry the relevant solutions are those corresponding to the isothermal sphere.

Collisional Equilibrium

We consider the collisional evolution of an N -body system further in a later subsection and here develop fundamental ideas about the isothermal model. The isothermal model has infinite mass, and much has been learned by considering a model confined within an adiabatic boundary or enclosure. There is a series of such models, characterized by a single dimensionless parameter, which can be taken to be the ratio between the central density and the density at the boundary, ρ_0/ρ_e (Figure 3).

These models are extrema of the Boltzmann entropy $S = -k \int f \ln f d^6\tau$, where k is the Boltzmann constant, and the integration is taken over all available phase space. Their stability may be determined by evaluating the second variation of S . It is found that it is negative definite, so that S is a local maximum and the configuration is stable, only if $\rho_0/\rho_e < 709$ approximately. A physical explanation for this is the following. In the limit when $\rho_0/\rho_e \simeq 1$, the self-gravity (which causes the spatial inhomogeneity) is weak, and the system behaves like an ordinary perfect gas. When $\rho_0/\rho_e \gg 1$, however, the system is highly inhomogeneous, consisting of a core of low mass and high density surrounded by an extensive halo of high mass and low density. Consider a transfer of energy from the deep interior to the envelope. In the envelope, which is restrained by the enclosure, the additional energy causes a rise in temperature, but this is small, because of the very large mass of the halo. Extraction of energy from around the core, however, causes the bodies there to sink and accelerate, and, because of the negative

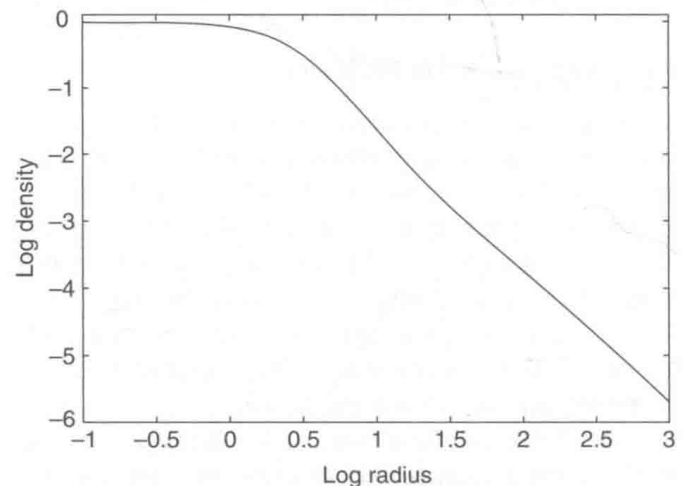


Figure 3 The density profile of the nonsingular isothermal model, with conventional scalings.

specific heat of a self-gravitating system, they gain more kinetic energy than they lost in the original transfer. Now the system is hotter in the core than in the halo, and the transfer of energy from the interior to the exterior is self-sustaining, in a gravothermal runaway. The isothermal model with large density contrast is therefore unstable.

The negative specific heat, and the lack of an equilibrium which maximizes the entropy, are two examples of the anomalous thermodynamic behavior of the self-gravitating N -body problem. They are related to the long-range nature of the gravitational interaction, the importance of boundary terms, and the nonextensivity of the energy. Another consequence is the inequivalence of canonical and microcanonical ensembles.

Numerical Methods

The foregoing considerations are difficult to extend to systems without a boundary, although they are a vital guide to the behavior even in this case. Our knowledge of such systems is due largely to numerical experiments, which fall into several classes:

1. Direct N -body calculations. These minimize the number of simplifying assumptions, but are expensive. Special-purpose hardware is readily available, which greatly accelerates the necessary calculations. Great care has to be taken in the treatment of few-body configurations, which otherwise consume almost all resources.
2. Hierarchical methods, including tree methods, which shorten the calculation of forces by grouping distant masses. They are mostly used for collisionless problems.
3. Grid-based methods, which are used for collisionless problems.
4. Fokker-Planck methods, which usually require a theoretical knowledge of the statistical effects of two-, three- and four-body interactions. Otherwise they can be very flexible, especially in the form of Monte Carlo codes.
5. Gas codes. The behavior of a self-gravitating system is simulated surprisingly well by modeling it as a self-gravitating perfect gas, rather like a star.

Collisional Evolution

Consider an isolated N -body system, which is supposed initially to be given by a spherically symmetric equilibrium solution of eqns [6] and [7], such as eqn [8]. The temperature decreases with increasing radius, and a gravothermal runaway causes the “collapse” of the core, which reaches

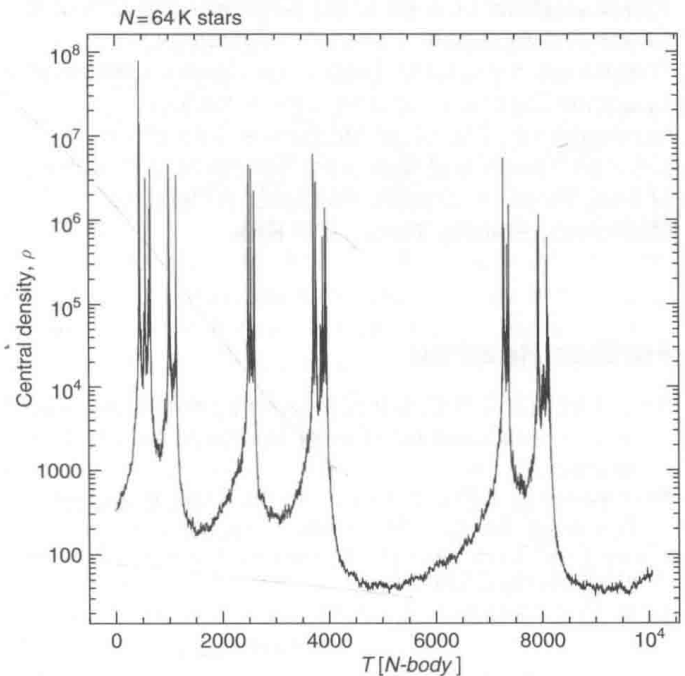


Figure 4 Gravothermal oscillations in an N -body system with $N = 65\,536$. The central density is plotted as a function of time in units such that $t_{cr} = 2\sqrt{2}$. (Source: Baumgardt H, Hut P, and Makino J, with permission.)

extremely high density in finite time. (This collapse takes place on the long two-body relaxation time-scale, and so it is not the rapid collapse, on a free-fall timescale, which the name rather suggests.)

At sufficiently high densities, the timescale of three-body reactions becomes competitive. These create bound pairs, the excess energy being removed by a third body. From the point of view of the one-particle distribution function, f , these reactions are exothermic, causing an expansion and cooling of the high-density central regions. This temperature inversion drives the gravothermal runaway in reverse, and the core expands, until contact with the cool envelope of the system restores a normal temperature profile. Core collapse resumes once more, and leads to a chaotic sequence of expansions and contractions, called gravothermal oscillations (Figure 4).

The monotonic addition of energy during the collapsed phases causes a secular expansion of the system, and a general increase in all timescales. In each relaxation time, a small fraction of the masses escape, and eventually (it is thought) the system consists of a dispersing collection of mutually unbound single masses, binaries, and (presumably) stable higher-order systems.

It is very remarkable that the long-term fate of the largest self-gravitating N -body system appears to be intimately linked with the three-body problem.

See also: Boltzmann Equation (Classical and Quantum); Chaos and Attractors; Dynamical Systems and Thermodynamics; KAM Theory and Celestial Mechanics; Lyapunov Exponents and Strange Attractors; Nonequilibrium Statistical Mechanics: Interaction between Theory and Numerical Simulations; Quantum N-Body Problem; Stability Problems in Celestial Mechanics; Stability Theory and KAM.

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Gravitational Waves

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In elementary physics presentations, one learns about electricity and magnetism, and also about gravity. There appear striking similarities between Newton's law of gravitational attraction and Coulomb's law of attraction between charges. There are also obvious differences, the most immediate one being that in gravitation all masses are positive and always attract each other, whereas in electromagnetism charges may attract or repel, depending on their signs. We also know today that Newton's theory of gravity is not considered an entirely correct description of the gravitational field, particularly when fields are time dependent and intense. The currently accepted theory of gravity is Einstein's theory of general relativity.

The similarity between electromagnetism and gravitation also holds to a certain extent when the fields depend on time. This is usually not discussed in elementary treatments since a full description of time-dependent gravitational fields requires the use of general relativity. It is true, however, that if the fields are weak, there exist several similarities between gravitation and electromagnetism. In particular, one can have waves in the gravitational field that are able to carry energy from a source to a receptor.

If one assumes that the metric of spacetime is close to the flat Minkowski metric $\eta_{\mu\nu}$, that is,

$g_{\mu\nu} = \eta_{\mu\nu} + h_{\mu\nu}$ with $|h_{\mu\nu}| \ll 1$ in Cartesian coordinates, the Einstein equations of general relativity, expanding to linear order in $h_{\mu\nu}$, become

$$\begin{aligned} 0 &= R_{\mu\nu} - \frac{1}{2} \eta_{\mu\nu} R \\ &= \frac{1}{2} (\partial_\sigma \partial_\nu h_{\mu}^\sigma + \partial_\sigma \partial_\mu h_{\nu}^\sigma - \partial_\mu \partial_\nu h \\ &\quad - \square h_{\mu\nu} - \eta_{\mu\nu} \partial_\mu \partial_\nu h^{\mu\nu} + \eta_{\mu\nu} \square h) \end{aligned} \quad [1]$$

These do not look like wave equations. However, if one chooses “harmonic coordinates,” $\square x^\mu = 0$, where \square is the d'Alembertian constructed with the full metric and then linearized, the vacuum Einstein equations become

$$\square h_{\mu\nu} = 0 \quad [2]$$

where \square is the d'Alembertian computed in the flat Minkowski metric.

Just as in electromagnetism the motion of charges produces waves, the motion of masses produces waves in the gravitational field. In the above wave equations, one would have nonzero right-hand sides if masses were present. In electromagnetism, the conservation of charge implies that the lowest order of “structure” a source must have to produce electromagnetic waves is that of a time-dependent dipole. In the gravitational field, the conservation of momentum implies that the lowest multipolar order of a source of gravitational waves must be a quadrupole. Moreover, gravity is a weaker force than electromagnetism when one considers usually available situations. One can exert forces of the orders of fractions of Newton with electromagnetic

charges easily collected in tabletop experiments. To produce similar amounts of gravitational force, one needs large quantities of mass. This last fact, coupled with the quadrupolar nature of the sources of gravitational waves, makes their production quite challenging in experimental terms. The luminosity of a gravitational wave source is given by the celebrated Einstein quadrupole formula,

$$L = \left(\frac{G}{5c^5} \right) \sum_{j,k=1}^3 \left(\ddot{I}_{jk} \right)^2 \quad [3]$$

where G is Newton's gravitational constant, c is the speed of light, and \ddot{I}_{ij} is the third-order time derivative of the traceless part of the quadrupole mass moment of the source.

Gravity is, however, a dominant force if one considers the universe at large (say, at least planetary) scales. There one would expect gravitational waves to play some role in the dynamics of the systems. In such systems, the presence of gravitational waves has indeed been experimentally confirmed. We know of a system of two pulsars in mutual orbit, PSR1913+16, whose orbit has been tracked with enough accuracy via radioastronomy to make the influence of gravitational waves observable. The motion of the pulsars makes the system an emitter of gravitational waves. Since the waves carry away energy, the orbit of the system decreases in radius and the period of oscillation increases. The system has now been tracked for over 20 years, and the prediction of the emitted amount of energy in gravitational waves due to general relativity has been confirmed with a very significant degree of accuracy. Penrose was the first to notice that if one considers how accurately Newton's theory plus the corrections due to general relativity predict the positions of the pulsars in their orbit, this is in fact the most accurately verified physical prediction ever.

Technically, even the existence of gravitational waves at a conceptual mathematical level, was an open problem for many years. Since the correct description of the waves is through the general theory of relativity, a "gravitational wave" should really be viewed as a "ripple in spacetime." Disentangling if such ripples are a true physical effect or a time-dependent coordinate transformation that propagates – to use the words of Eddington – "with the speed of thought" took quite a bit of technical development within the general theory of relativity. It was only in the 1960s that a clear enough conceptual picture was developed to determine that gravitational waves were indeed a true physical phenomenon akin to electromagnetic waves. And in

particular that one can unambiguously characterize them as transporting energy, momentum, and angular momentum from a source to an observer.

Gravitational waves are as difficult to detect as they are to produce. Since all masses fall in the same way in a gravitational field, one needs to couple to the gradients of the field to detect gravitational waves, which diminishes the efficiency. Attempting to produce gravitational waves via mechanical means in the lab (e.g., by rotating a bar of metal) produces too little luminosity, and in addition, the relatively low frequency implies that the wave zone is far away, which further decreases the chances for detection. Up to date, no one has succeeded in producing a Hertz-like experiment for gravitational waves and the jury is still out on the issue if future technologies (e.g., the use of superconductors to produce waves of gigahertz frequency) will ever allow such an experiment.

Efforts to attempt to detect gravitational waves produced by astrophysical phenomena started in the 1960s with pioneering work by Weber. The initially proposed technology for detection was the construction of large (~ 1 ton) resonant bars. The idea was to use sensitive technology to measure the resonance of the bar as gravitational waves of astrophysical origin impact on it. Gravitational waves manifest themselves as a stretching and contraction of lengths. The contraction or stretching is proportional to the length of the object considered and is therefore characterized by a dimensionless number, the "strain" $\Delta L/L$ usually called " h ." Conservative current estimates of possible astrophysical sources state that on Earth one should not expect strains larger than 10^{-22} for events that repeat more frequently than a few times every year. Detectors with bar technology are approaching their fundamental quantum limits with strains that appear to be too large for detection to be ensured. This led to the proposal of a new technology, the use of Michelson-type interferometers to detect the waves. Currently, several interferometric detectors are being built in the US, Europe, Japan, and Australia that expect to achieve enough sensitivity for detection within a few years. Contrary to the bars, which are quintessentially narrow-band detectors (most bars operate ~ 900 Hz with a bandwidth of ~ 10 Hz), interferometric detectors are broadband. Current detectors have a sensitivity curve limited by various sources of noise that make them suitable for detection within the 10 Hz–1 kHz band. The broadband nature of the detectors opens several opportunities for the use of data analysis techniques that can allow the detection of gravitational waves that have strains even lower than the noise of the detectors. Moreover, several of

the candidate events “evolve” in frequency as they emit gravitational waves (in the case of the binary pulsar, for instance, the frequency “sweeps up” as the system loses energy), and such evolution could be monitored with interferometric detectors. This would allow several insights into the physics of the observed systems.

An important limitation of any type of detector based on Earth is that the seismic noise increases quite significantly below 10 Hz. Even if seismic isolation allowed sensitivities below 10 Hz, gravity gradients due to Earth’s seismic motion and due to clouds would limit ground-based detectors to 1 Hz and above. The frequency at which a system emits gravitational waves is inversely proportional to the system’s mass (a simple way to see this is to realize that larger systems move proportionally slower to their size). However, larger systems generically have more mass and therefore consequently emit larger amounts of energy in gravitational waves. This suggests that setting up detectors in space, free of the constraints of seismic noise, would offer significant promise in detecting gravitational waves. Currently, there is a proposal for a space-borne gravitational wave detector consisting of three satellites in a solar orbit that trails that of Earth. Lasers would be sent between the satellites to track their relative positions, which will be separated by 5 million kilometers. Such a detector would be sensitive in frequencies of 10^{-4} – 10^{-2} Hz. In such a frequency band, one expects that compact objects plunging into supermassive black holes and other sources will be readily available. Detection of gravitational waves on Earth is considered marginal, in the sense that conservative current estimates cannot guarantee that there will be enough events to make the detection successful at significant event rates. Conversely, for the detectors in space, detection should be guaranteed at high event rates.

Possible sources of gravitational waves to be detected by the Earth-based interferometric detectors are:

1. Binary systems of compact objects. As the system orbits, it emits gravitational waves, which makes the orbit shrink in size and the orbiting period shorter with the objects eventually merging together. Potential systems include black hole binaries, neutron star binaries and mixed black hole/neutron star binaries. As the system sweeps up in orbital speed towards the merger, so does the frequency of the gravitational waves emitted. For binaries of neutron stars, which usually have masses slightly larger than the mass of the Sun, the last few minutes of the binary inspiral will be
2. detectable by the current generation of gravitational wave detectors, up to a distance of several mega-parsecs for the initial detectors, increasing to a few hundreds of mega-parsecs for improvements planned for the next few years. For black hole binaries, since the masses can be larger, one expects larger signal-to-noise ratio for the same distance or to be able to detect at larger distances.
2. Spinning neutron stars that develop “mountains” or other irregularities in the surface would produce gravitational waves of small amplitude but of a very regular periodic nature. This makes them prime candidates for data analysis techniques that could exhibit the presence of the wave even though it is weaker than the background noise of the interferometers. Integration periods of several months may be needed for detection, depending on the size of the asymmetries in the neutron stars.
3. Supernovas or other violent events are obviously possible sources of gravitational waves. However, the quadrupole nature of the waves requires the events to be asymmetric in order to produce gravitational waves. Current numerical models of supernovas are not accurate enough to predict in a clear way the level of asymmetry to make reliable predictions of how frequently and at what intensity could these types of sources be detected.
4. The primordial background of gravitational waves produced in the big bang is not expected to be detectable by the Earth-based detectors. The precise amplitude of the background is unknown, depending on details of cosmological models. The detectors are likely to be able to constrain some of the models that predict large amplitudes for the gravitational wave background.

For the space-based detectors, the situation is more favorable, since there exist sources of gravitational waves that are guaranteed to be detected. Potential sources of gravitational waves are:

1. *Merger of the supermassive black holes at the centers of two galaxies.* Given the large amounts of mass involved, they would be easily detected and very precise measurements of the system’s parameters and of various general relativistic behaviors could be possible. Such systems should be detectable all across the universe, although it is not expected that such systems form for redshifts larger than 30.
2. *Inspiral of compact objects into the supermassive black holes at the centers of galaxies* (neutron

stars, white dwarfs, solar-sized black holes). These processes will allow the usage of gravitational waves to map precisely the gravitational field of the supermassive object.

3. *White-dwarf binaries and low-mass X-ray binaries.* There exist about a dozen such systems optically observable with gravitational wave frequencies above 0.1 mHz that the space-based detectors should be able to detect. There is likely to be a large population of other systems that are also detectable and are not optically visible. In fact, there may be so many of these sources that time resolution would be impossible, and they would form a random background.
4. *Collapse of supermassive stars.* The formation mechanism for the supermassive black holes in the centers of galaxies is still uncertain. One possibility is that they stem from the collapse of supermassive stars, and in that case a potentially significant emission of gravitational waves could take place.
5. *Primordial background of gravitational waves.* Unfortunately, the abundance of white-dwarf binaries as a source is expected to cloud the ability of the space detectors to observe primordial gravitational waves in an important portion of the spectrum of the instrument, although it appears possible at low frequencies, where it could compete with the bounds set by pulsar timing.

The current Earth-based gravitational wave projects include the LIGO project in the US, funded by the National Science Foundation and jointly operated by Caltech and MIT and a consortium of institutions known as the LIGO Science Collaboration. LIGO consists of two 4 km long Fabry–Perot recycled Michelson interferometers, one in Hanford, WA, and one in Livingston, LA. In Europe, the GEO600 project is a 600 m dual-recycled interferometer near Hanover in Germany and the Virgo project is a 3 km interferometer near Pisa in Italy operated by a French–Italian consortium with a similar optical configuration as LIGO. TAMA300 is a 300 m interferometer in Japan also with the same configuration as LIGO. When all these detectors are in operation, sources seen in coincidence could be localized by triangulation. TAMA is now operating close to design sensitivity, GEO600 and LIGO are likely to operate at design sensitivity in 2006, with VIRGO following close behind. The space-based interferometer project is called the LISA project and is planned as a joint NASA/ESA project. ESA has approved a launching date for 2015, but it is plausible that the mission could be launched at an earlier date.

A direct detection of gravitational waves would be a breakthrough in experimental science, as well as a confirmation of the dynamic nature of gravity in general relativity. Once the detection of gravitational waves becomes a routine matter, one can imagine a revolution in astronomy as one uses gravitational waves to “see” the universe. Since they are so hard to produce and interfere with, gravitational waves become an excellent type of “light” to look at the universe with. Gravitational waves will be produced by important concentrations of mass, correlating well with “interesting” astronomical processes, and is not expected to be affected by the presence of dust or other interfering objects that could easily obscure electromagnetic waves. In addition to this, one has several “standard candles” for gravitational waves (e.g., most neutron stars have masses that differ by a few percent from 1.4 solar masses). This could allow, for instance, to determine with a high degree of accuracy the Hubble constant. Gravitational waves will also provide insight into the nuclear equation of state that holds in the interior of compact objects like neutron stars. Contrary to ordinary electromagnetic radiation, which “decoupled” from matter only when the universe became cool enough after the big bang, gravitational waves could be used to probe the universe further into the past. The detection could also prove that gravitational waves travel at the speed of light, a prediction of general relativity and other theories.

An interesting observation is that most astrophysical objects that are quite visible in the electromagnetic spectrum are unlikely to be visible in terms of gravitational waves, and vice versa. This makes the information we will gather from gravitational wave astronomy complementary to what we learn from optical (electromagnetic) astronomy. Moreover, it should be noted that wavelengths of electromagnetic waves are typically very small compared to the size of the astronomical objects they depict. This is due to the fact that the waves are really not produced by the objects themselves but by atoms on the surface of the objects or in regions nearby, usually very hot and in gaseous form. In contrast, gravitational waves are produced by the bulk matter of astronomical objects and their wavelengths are expected to be long as compared to the objects that produce them. They are more akin to a sound than to light in this respect, another reason to suspect that the information we will get from them is unlike any information obtained electromagnetically.

Gravitational waves are likely to bring great surprises. Every time a new window has been opened on the universe – for instance, the use of radio waves – our view of the universe has been revolutionized. Given how differently they operate

at a detailed level with respect to radio waves, the surprises from gravitational waves used as tools to view the universe are potentially even greater.

See also: Asymptotic Structure and Conformal Infinity; Computational Methods in General Relativity: The Theory; General Relativity: Experimental Tests; General Relativity: Overview.

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- The LIGO project web page, which includes links to all the other experimental efforts: <http://www.ligo.caltech.edu>.

Growth Processes in Random Matrix Theory

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Introduction

Probability distributions coming from random matrix theory (RMT), RMT laws, occur in different contexts, notably in quantum physics and in number theory. RMT laws are also seen in certain local random growth models and related problems in discrete probability, random permutations, exclusion processes, and random tilings (dimer models). In these models limit laws for height/shape fluctuations are given by limit laws from RMT, in particular the largest eigenvalue or Tracy–Widom distributions. These models belong to the Kardar–Parisi–Zhang (KPZ) universality class. Models in this class have two universal exponents, $1/3$ describing the interface fluctuations and $2/3$ describing the correlations in the transversal direction. By a local random growth model, we mean a model where the random growth mechanism is local in that it does not depend on the global geometry as in diffusion limited aggregation (DLA). Typically there is also some smoothing mechanism. The connection with RMT can only be established for special exactly solvable models. Below we discuss a basic model based on a last-passage percolation problem, which translates into a polynuclear growth (PNG) process. Other models that can be treated are in a sense variations of this model. Point processes with determinantal correlation functions play a central role in RMT and in the analysis of the basic model and we start by discussing these. The basic

model has several different interpretations that will be outlined. Another basic tool, which can be formulated in different ways, is the Robinson–Schensted–Knuth (RSK) correspondence well known in combinatorics. One approach is in terms of nonintersecting paths which translates into a multilayer PNG process. Limit theorems can be formulated for the height above a fixed location, and also for the whole height function in terms of the Airy process which extends the Hermitian Tracy–Widom distribution F_2 . It is expected that several results should generalize to a broader class of models. There is a natural universality problem of extending the validity of the RMT laws.

Determinantal Processes

Point processes with determinantal correlation functions play an important role in the exactly solvable models. We consider probability measures on $\Lambda^n, \Lambda \subseteq \mathbb{R}$, of the form

$$\frac{1}{Z_n} \det(\phi_i(x_j))_{i,j=1}^n \det(\psi_i(x_j))_{i,j=1}^n d^n \mu(x) \quad [1]$$

which can be thought of as describing random points in Λ at positions x_1, \dots, x_n . Here, μ is a reference measure on Λ , for example, Lebesgue or counting measure, Z_n a normalization constant, and ϕ_i, ψ_i given functions. A measure of this form has determinantal correlation functions in the sense that the density, with respect to $d^m \mu(y)$, of particles at y_1, \dots, y_m is

$$\rho(y_1, \dots, y_m) = \det(K_n(y_i, y_j))_{i,j=1}^m \quad [2]$$

There is an explicit formula for the correlation kernel K_n in terms of the functions ϕ_i, ψ_i .

The eigenvalue measures in the basic random matrix ensembles have the form

$$\frac{1}{Z_n} |\Delta_n(x)|^\beta \prod_{j=1}^n w(x_j) d^n \mu(x) \quad [3]$$

where $\Delta_n(x) = \det(x_j^{i-1})_{i,j=1}^n$ is Vandermonde's determinant, $x \in \Lambda^n$ and x_1, \dots, x_n are the eigenvalues. For the Gaussian unitary ensemble (GUE_n), $Z_n^{-1} \exp(-\text{tr } M^2) dM$ of $n \times n$ Hermitian matrices M , we have $\beta=2$, $\Lambda=\mathbb{R}$, $w(x)=\exp(-x^2)$ and μ the Lebesgue measure. For the Laguerre unitary ensemble ($\text{LUE}_{n,\nu}$) of complex covariance matrices, $M^* M$, where M is an $(n+\nu) \times n$ -matrix with standard complex Gaussian elements, we have $w(x)=x^\nu e^{-x}$, $\nu \geq 0$, $\beta=2$, $\Lambda=[0, \infty)$ and μ the Lebesgue measure. The $\beta=2$ case of [3] can be put into the form [1] and hence has determinantal correlation functions. In this case the correlation kernel can be expressed in terms of the normalized orthogonal polynomials $p_k(x)$ with respect to $w(x) d\mu(x)$ on Λ . Because of this when $\beta=2$ the ensemble [3] is referred to as an orthogonal polynomial ensemble (OPE). The kernel is given by

$$K_n(x, y) = \sum_{k=0}^{n-1} p_k(x) p_k(y) (w(x) w(y))^{1/2} \quad [4]$$

A consequence of [2] is that the probability of finding no particle in a set $J \subseteq \Lambda$ is given by a Fredholm determinant,

$$\mathbb{P}[\text{no particle in } J] = \det(I - K_n)_{L^2(J, \mu)} \quad [5]$$

In particular the distribution function $F(\xi)$ of the largest eigenvalue or rightmost particle $x_{\max} = \max_{1 \leq j \leq n} x_j$ in an OPE is given by [5] with K_n as in [4] and $J = (\xi, \infty)$.

A Basic Model

Let $(w(i, j))_{(i, j) \in \mathbb{Z}_+^2}$ be independent geometric random variables with parameter $a_i b_j$,

$$\mathbb{P}[w(i, j) = k] = (1 - a_i b_j)(a_i b_j)^k \quad [6]$$

$k \geq 0$ and $0 \leq a_i b_j < 1$. As a limiting case we can obtain exponential random variables. Consider the last-passage time

$$G(M, N) = \max_{\pi} \sum_{(i, j) \in \pi} w(i, j) \quad [7]$$

where the maximum is over all up/right paths π from $(1, 1)$ to (M, N) , that is, $\pi = \{(i_1, j_1), \dots, (i_m, j_m)\}$ with $(i_{k+1}, j_{k+1}) - (i_k, j_k) = (1, 0)$ or $(0, 1)$, $(i_1, j_1) = (1, 1)$ and $(i_m, j_m) = (M, N)$, $m = M + N - 1$. We can also think of this as a zero-temperature directed

polymer, by thinking of the $w(i, j)$'s as (minus) energies and π as random walk paths.

As will be explained in some more detail below, if the $w(i, j)$'s are exponential with mean 1 and $M \geq N$, then $G(M, N) = \lambda_{\max}$ in distribution, $M \geq N$, where λ_{\max} is the largest eigenvalue in $\text{LUE}_{N, M-N}$. Hence, in this case $G(M, N)$ behaves exactly like a largest eigenvalue. If the $w(i, j)$'s are geometric with parameter q , then $G(M, N)$ has the same distribution as the rightmost particle in an OPE, namely [3], with $\beta=2$, $w(x) = \binom{M-N+x}{x} q^x$ and μ the counting measure on $\Lambda = \mathbb{N}$, called the Meixner ensemble. Since in this case the relevant orthogonal polynomials are discrete the ensemble is referred to as a discrete OPE.

The random variables $\{G(M, N)\}_{(M, N) \in \mathbb{Z}_+^2}$ have two interpretations related to random growth. It follows from [7] that

$$\begin{aligned} G(M, N) &= \max(G(M-1, N), G(M, N-1)) \\ &\quad + w(M, N) \end{aligned} \quad [8]$$

This can be thought of as a growth rule. We change variables by letting $G(M, N) = h(M-N, M+N-1)$ and $w(M, N) = \omega(M-N, M+N-1)$ with $w(M, N) = 0$ if $(M, N) \notin \mathbb{Z}_+^2$. Then

$$\begin{aligned} h(x, t+1) &= \max(h(x-1, t), h(x, t), h(x+1, t)) \\ &\quad + \omega(x, t) \end{aligned} \quad [9]$$

$x \in \mathbb{Z}$, $t \in \mathbb{N}$, $h(x, 0) \equiv 0$, and $\omega(x, t) = 0$ if $|x| \geq t$ or if $x-t$ is even. We can extend it to the whole real line by letting $h(x, t) = h([x], t)$. The growth rule [9] is a discrete polynuclear growth (PNG) model. Up-steps in the interface, $x \rightarrow h(x, t)$ (see the top curve in Figure 1), move at unit speed to the left and down-steps move at unit speed to the right and they merge at collision. On top of this smoothing mechanism, we have random deposition given by $\omega(x, t)$. Looking at the definition of ω , we see that all deposition up to time t is on top of a basic layer $(-t, t)$. The asymptotic shape will look like a droplet and this setting of PNG is called the droplet geometry. We see that height fluctuations are directly related to fluctuations of $G(M, N)$.

We get another growth model, the corner growth model, somewhat similar to the classical Eden growth model, by considering the random shape (see Figure 2),

$$\begin{aligned} \Omega(n) &= \{(M, N) \in \mathbb{Z}_+^2; G(M, N) + M + N - 1 \leq n\} \\ &\quad + [-1, 0]^2 \end{aligned} \quad [10]$$

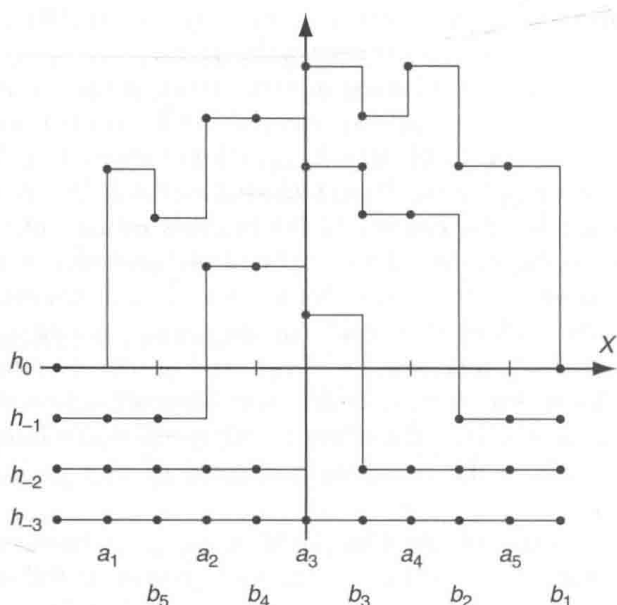


Figure 1 Multilayer PNG model.

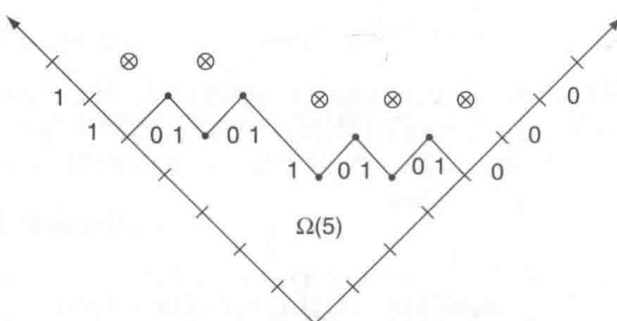


Figure 2 Corner growth model at time $n=5$. The crosses are the possible growth sites.

The complement of this set in \mathbb{Z}_+^2 has a boundary $B(n)$ which we can think of as an interface. By [8] and the lack of memory property of the geometric/exponential distribution, the region $\Omega(n)$ grows by adding new squares independently at each corner of $B(n)$ with geometric/exponential waiting times (see Figure 2). If we look at $B(n)$ in a coordinate system with $M=N$ as vertical axis and write a 1 for every unit down-step on $B(n)$ and a 0 for every unit up-step (see Figure 2), the corner growth dynamics translates into the totally asymmetric simple exclusion process (TASEP), in discrete or continuous time, with initial configuration $\dots 1111000\dots$. As shown by Jockush, Propp, and Shor, $\Omega(n)$ also occurs in a uniform random domino tiling of a region called the Aztec diamond (see Figure 3). The shape $\Omega(n)$, when $q=1/2$, has the same law as the completely regular (frozen) North Polar Region (NPR) in the tiling and hence the boundary fluctuations of the NPR are related to the fluctuations of $G(M, N)$. The NPR in Figure 3 has the same

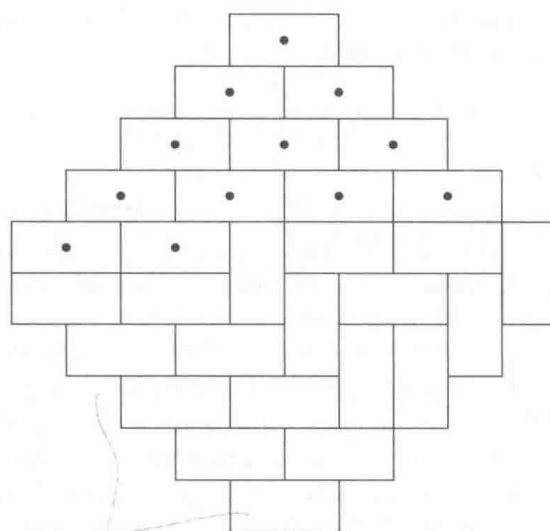


Figure 3 Domino tiling of an Aztec diamond of size $n=5$. Dominoes marked by dots form the NPR.

shape as $\Omega(5)$ in Figure 2. This connects the models considered here with dimer or tiling problems in two-dimensional equilibrium statistical mechanics.

Consider a (Poissonized) random permutation σ from S_N , where N is a $\text{Poisson}(\alpha)$ random variable. Let $L(\alpha)$ denote the length of the longest increasing subsequence in σ , for example, $\sigma=316452$ has $L=3$. By thinking of the representation of a permutation by its permutation matrix, we see that $G(N, N)$ with $w(i, j)$ geometric with parameter $q=\alpha/N^2$ converges to $L(\alpha)$ in distribution as $N \rightarrow \infty$. We call this limit the Poisson limit. Taking this limit in the PNG process yields the Prähofer–Spohn continuous time PNG (cont-PNG) model, which is similar to the discrete PNG defined above but where all steps have unit size and we have continuous time dynamics with deposition events according to a two-dimensional spacetime Poisson process. The study of $L(\alpha)$, and its de-Poissonization when N is nonrandom, is known as Ulam's problem in combinatorial probability.

The RSK Correspondence

The mapping of the last-passage problem [7] into a determinantal process is based on the RSK correspondence. This correspondence maps the integer matrix $(w(i, j))_{1 \leq i, j \leq M}$ bijectively to a pair of semi-standard Young tableaux (P, Q) with common shape λ , which is a partition $\lambda=(\lambda_1, \lambda_2, \dots)$ of $\sum_{1 \leq i, j \leq M} w(i, j)$. This map has the property that $G(M, N)=\lambda_1$, the length of the first row in the Young diagram. From the combinatorial definition of the Schur polynomials s_λ it follows that the measure [6] on the integer matrix is mapped to a

probability measure on partitions, the Schur measure, given by

$$P_{\text{Schur}}[\lambda] = \frac{1}{Z} s_{\lambda}(a_1, \dots, a_M) s_{\lambda}(b_1, \dots, b_M) \quad [11]$$

This measure has determinantal correlation functions if we think of $x_i = \lambda_i - i$ as the positions of particles in \mathbb{Z} . If we use $x_i = \lambda_i + N - i$ as variables and specialize to $a_1 = \dots = a_M = \sqrt{q}$, $b_1 = \dots = b_N = \sqrt{q}$ and $b_j = 0$ for $j > N$ we get the Meixner ensemble. The case of exponential random variables, for example the relation to LUE discussed above, is obtained from the Meixner ensemble by taking an appropriate limit. In the Poisson limit we get the Poissonized Plancherel measure,

$$P_{\text{Plan}}^{\alpha}[\lambda] = \sum_{N=0}^{\infty} \frac{e^{-\alpha/\alpha^n}}{N!} \quad [12]$$

where $P_{\text{Plan},N}[\lambda] = (\dim \lambda)^2/N!$ if λ is a partition of N and 0 otherwise. Here $\dim \lambda$ is the dimension of the irreducible representation of S_N labeled by λ . In the work of Borodin and Olshanski in representation theory various measures on partitions with determinantal correlation functions occur naturally. Also Okounkov and co-workers have used the Plancherel and Schur measures in Gromov–Witten theory. The correlation kernel for the Plancherel measure represented as the point process $(x_i)_{i \geq 1}$ in \mathbb{Z} with $x_i = \lambda_i - i$ has the correlation kernel, called the discrete Bessel kernel,

$$B^{\alpha}(x, y) = \sqrt{\alpha}(x - y)^{-1} \times (J_x(2\sqrt{\alpha})J_{y+1}(2\sqrt{\alpha}) - J_{x+1}(2\sqrt{\alpha})J_y(2\sqrt{\alpha})) \quad [13]$$

where J_n is the ordinary Bessel function. The random variable $L(\alpha)$ has the same distribution as $\max x_i + 1$. Hence, by [5],

$$P[L(\alpha) \leq n] = \det(I - B^{\alpha})_{\ell^2(\{n, n+1, \dots\})} \quad [14]$$

The random variable $L(\alpha)$ also gives the height above the origin in cont-PNG.

There is a geometric interpretation of RSK going back to Viennot. The pair (P, Q) is represented as a family of nonintersecting paths in a directed graph. These paths can be obtained by running a multilayer version of the PNG process where the size of collisions are deposited as growth in lower layers which evolve according to the same PNG dynamics. The information lost in the collisions is recorded in the lower layers. This can be done also for $\{w(i, j)\}_{i+j-1 \leq t}$ and leads to a multilayer version of [9], $\{h_{-j}(x, t)\}_{j=1}^{\infty}$, where $h_{-j}(x, 0) \equiv -j$, $h_{-j}(\pm t, t) = -j$, and $h(x, t) = h_0(x, t)$ is the top path (see Figure 1).

The Karlin–McGregor theorem or the Gessel–Viennot method say that the weight (probability) of a family of nonintersecting paths with fixed initial and final positions on a weighted directed acyclic graph is given by a determinant. It follows that the probability of a certain configuration $\{h_{-j}(0, t)\}_{j \geq 1}$ is given by a product of two determinants and hence has the form [1]. In Figure 1, the weights of the horizontal line segments will be 1, whereas each unit vertical step has weight a_i or b_j as indicated in the figure. This leads to [9] using the Jacobi–Trudi formula for the Schur polynomial.

Limit Theorems

The existence of a limit shape in a model like [6] with $w(i, j)$ independent random variables, and in related problems follows by a subadditivity argument, although explicit shapes are only known in a few cases. The formalism described above makes it possible to get more detailed results about the fluctuations around the limit shape, like a central-limit theorem, but with a non-normal limit law. We know that $G(M, N)$ has the same distribution as $x_{\max} - N + 1$, where x_{\max} is the rightmost particle in the Meixner ensemble. This, together with [4], [5], and an asymptotic analysis of the Meixner polynomials, gives

$$P[G(M, N) \leq w(\gamma, q)N + \xi \sigma(\gamma, q)N^{1/3}] \rightarrow F_2(\xi) \quad [15]$$

as $N \rightarrow \infty, M \rightarrow \infty, M/N \rightarrow \gamma \geq 1$, where

$$w(\gamma, q) = \frac{(1 + \sqrt{q\gamma})^2}{1 - q} - 1 \quad [16]$$

and

$$\sigma(\gamma, q) = \frac{(q/\gamma)^{1/6}}{1 - q} (\sqrt{\gamma} + \sqrt{q})^{2/3} (1 + \sqrt{q\gamma})^{2/3} \quad [17]$$

The limiting distribution function F_2 is the Tracy–Widom distribution given by

$$F_2(\xi) = \det(I - A)_{L^2(\xi, \infty)} \quad [18]$$

where

$$A(x, y) = \frac{\text{Ai}(x)\text{Ai}'(y) - \text{Ai}'(x)\text{Ai}(y)}{x - y} \quad [19]$$

is the Airy kernel. It is also the limiting largest eigenvalue distribution for GUE_n ,

$$\lim_{N \rightarrow \infty} P \left[\frac{\sqrt{2n} \lambda_{\max}^{(n)} - 2n}{n^{1/3}} \leq \xi \right] = F_2(\xi) \quad [20]$$

The function F_2 can also be expressed in terms of a Painlevé II function. The limit theorem [15]

translates into a fluctuation result for the height function in the corner growth and the PNG models, saying that the height fluctuations above a fixed location at time t are of order $t^{1/3}$ and given by the F_2 -distribution. Here we see the KPZ exponent $1/3$.

For the length $L(\alpha)$ of the length of a longest increasing subsequence in a random permutation or the height above the origin in the cont-PNG, [14] and asymptotics for Bessel functions yield

$$\mathbb{P}[(L(\alpha) - 2\sqrt{\alpha})/\alpha^{1/6} \leq \xi] \rightarrow F_2(\xi) \quad [21]$$

as $\alpha \rightarrow \infty$. This result was first proved by Baik, Deift, and Johansson using a Toeplitz determinant formula (Gessel's formula) for the left-hand side of [14] and the Deift–Zhou nonlinear steepest descent method for oscillatory Riemann–Hilbert problems. The above limit theorems can be extended to limit theorems for the whole point process rescaled around the rightmost point. This results in a limiting determinantal point process given by the Airy kernel [19].

The Airy Process

From the point of view of the growth processes, for example, the PNG process [7], it is natural to consider a scaling limit of the whole height function $x \rightarrow h(x, t)$ as $t \rightarrow \infty$. Looking at the height configuration in the multilayer growth process $x \rightarrow \{h_{-j}(x, t)\}_{j \geq 1}$ at different locations $x_1, \dots, x_r, x_{r+1}, \dots, x_{M-1}$ leads, via the Karlin–McGregor or Gessel–Viennot method, to probability measures of the form

$$\frac{1}{Z} \prod_{r=0}^{M-1} \det \left(\phi_{r,r+1} \left(y_i^r, y_j^{r+1} \right) \right)_{i,j=1}^n \quad [22]$$

with y^0 and y^M fixed configurations. Here, in the discrete PNG model, $\phi_{r,r+1}(x, y)$ is the transition probability (weight) to go from height x to height y between positions x_r and x_{r+1} . This measure generalizes [1] and it also has determinantal correlation functions. Measures of this form also arise in multimatrix models and in Dyson's Brownian motion model, $t \rightarrow M(t), t \in \mathbb{R}$, for Hermitian matrices, which is a Gaussian multimatrix model. The elements of the time-dependent Hermitian matrix $M(t)$ evolve according to independent Ornstein–Uhlenbeck processes and we have the transition kernel

$$Z^{-1} \exp[-\text{tr}(M(t) - qM(0))^2/(1 - q^2)] \quad [23]$$

where $q = \exp(-t)$. This process has GUE as its stationary distribution. The Harish–Chandra/Itzykson–Zuber integral can be used to show that the joint eigenvalue measure for $M(t_1), \dots, M(t_{M-1})$ has the

form [22] and hence has determinantal correlation functions. The correlation kernel is the extended Hermite kernel,

$$K_n(\tau, x; \sigma, y) = \begin{cases} \sum_{k=1}^{\infty} e^{-k(\tau-\sigma)} p_{n-k}(x) p_{n-k}(y) e^{-\frac{1}{2}(x^2+y^2)} & \text{if } \tau \geq \sigma \\ - \sum_{k=-\infty}^0 e^{-k(\tau-\sigma)} p_{n-k}(x) p_{n-k}(y) e^{-\frac{1}{2}(x^2+y^2)} & \text{if } \tau < \sigma \end{cases} \quad [24]$$

with p_k the normalized Hermite polynomials, $p_k \equiv 0$ if $k < 0$. Notice that this reduces to the Hermite kernel [4] when $\tau = \sigma$. This machinery can be used to show that the largest eigenvalue process $t \rightarrow \lambda_{\max}^{(n)}(t)$ induced by $M(t)$ converges in the sense of finite-dimensional distributions to a limiting process, the Airy process,

$$(\sqrt{2n} \lambda_{\max}^{(n)}(n^{-1/3}t) - 2n)/n^{1/3} \rightarrow \mathcal{A}(t) \quad [25]$$

as $n \rightarrow \infty$. The Airy process $\mathcal{A}(t)$, which is a stationary process, can be viewed as the top curve of a multilayer process $t \rightarrow (\mathcal{A}_{-j}(t))_{j \geq 1}$, $\mathcal{A}(t) = \mathcal{A}_0(t)$ such that the point process $\{\mathcal{A}_{-j}(t_k)\}_{1 \leq k \leq M, j \geq 0}$ has determinantal correlation functions with correlation kernel

$$A(\tau, \xi; \tau', \xi') = \begin{cases} \int_0^{\infty} e^{-\lambda(\tau-\tau')} \text{Ai}(\xi + \lambda) \text{Ai}(\xi' + \lambda) d\lambda & \text{if } \tau \geq \tau' \\ - \int_{-\infty}^0 e^{-\lambda(\tau-\tau')} \text{Ai}(\xi + \lambda) \text{Ai}(\xi' + \lambda) d\lambda & \text{if } \tau < \tau' \end{cases} \quad [26]$$

the extended Airy kernel, which reduces to the ordinary Airy kernel [19] when $\tau = \tau'$. The Airy process can be viewed as an extension of the Tracy–Widom distribution F_2 . For the PNG model above, the multilayer process is described by an extended kernel, which in the cont-PNG is an extended version of the discrete Bessel kernel [13]. In a suitable scaling limit, this extended kernel converges to the extended Airy kernel. For the PNG process [7], this leads to the limit law

$$(dN^{1/3})^{-1} \left[h \left(2d^{-1} \frac{1 + \sqrt{q}}{1 - \sqrt{q}} N^{2/3} \tau, 2N - 1 \right) - \frac{2\sqrt{q}}{1 - q} N \right] \rightarrow \mathcal{A}(\tau) \quad [27]$$

as $N \rightarrow \infty$, where $d = (1 - q)^{-1}(\sqrt{q})^{1/3}(1 + \sqrt{q})^{1/3}$. Notice the exponent $2/3$ which is the second KPZ exponent. This exponent can also be seen in the transversal fluctuations of the maximal paths in [6] for $G(N, N)$. These are superdiffusive, they have fluctuations of order $N^{2/3}$ around the diagonal, compared to $N^{1/2}$ for random walk paths between the same points. A fluctuation result like [27] can also be proved for the corner growth model and hence also for the Aztec diamond. The boundary of the NPR suitably rescaled converges to the Airy process.

Variations

Above we discussed one possible geometry, the droplet, for the PNG process. If we start with $h(x, 0) \equiv 0$ and allow random depositions along the whole line, we get an interface that is macroscopically flat, and not curved as in the droplet case. In this case, the height fluctuations above a fixed location at time t are again of size $t^{1/3}$ and described by the Gaussian Orthogonal Ensemble largest eigenvalue distribution. This law comes from the scaling limit of the rightmost particle in [3] with $\beta = 1$, $w(x) = \exp(-x^2)$, $\Lambda = \mathbb{R}$, and μ the Lebesgue measure. In this case, the correlation functions are not determinants but rather pfaffians. The result for flat PNG follows from the Baik–Rains analysis of symmetrized last-passage or permutation problems. In the PNG model we can also consider an interface in equilibrium. This can be put into the last-passage percolation picture by suitable boundary conditions, different parameters for $w(i, j)$ when i or j equals 1 or extra Poisson points on the axes in the Poisson limit. Results by Baik and Rains show that in the cont-PNG in equilibrium the height fluctuations are given by a relative of the Tracy–Widom distribution, F_0 . In these last two cases, the scaling limit of the whole height profile is not known.

The types of results discussed above can only be obtained for very special models. However, it is expected that many of the results (in particular the KPZ exponents $1/3$ and $2/3$, and also the fluctuation laws, including the Airy process) should generalize

to many other models. The different interpretations of [6] mentioned above suggest different generalizations, various local growth models, directed polymers, asymmetric exclusion processes, and dimer/tiling problems. RMT laws are natural limit laws for which the domain of attraction is not understood.

See also: Combinatorics: Overview; Determinantal Random Fields; Dimer Problems; Integrable Systems in Random Matrix Theory; Random Walks in Random Environments; Random Matrix Theory in Physics; Random Partitions.

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Hamiltonian Fluid Dynamics

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Introduction

The ideal fluid description is one in which viscosity or other phenomenological terms are neglected. Thus, as is the case for systems governed by Newton's second law without dissipation, such fluid descriptions possess Lagrangian and Hamiltonian descriptions. In fact, in the eighteenth century, Lagrange himself discussed what is in essence the action principle for the incompressible fluid. The subsequent history of action functional and Hamiltonian formulations of the ideal fluid is long and convoluted with contributions from Clebsch in the nineteenth century, and the likes of L Landau and V Arnol'd in the mid-twentieth century. In the early 1980s, there was a flurry of activity on the noncanonical Poisson bracket formulation, and this formulation is the focus of the present treatment, which is motivated by the work of the author, D Holm, J Marsden, T Ratiu, A Weinstein, and others.

Noncanonical Hamiltonian Structure

The traditional arena for Hamiltonian dynamics is the cotangent bundle $\mathcal{M} := T^*Q$, the phase space, which is naturally a symplectic manifold with a closed non-degenerate 2-form. In coordinates, the 2-form is given by $\omega_c = dq \wedge dp$, where q denotes the configuration coordinate for the base space manifold Q and p denotes the corresponding canonical momenta that arise from Legendre (convex) transformation. The 2-form ω_c provides a natural identification at a point $z = (q, p) \in \mathcal{M}$ of $T_z^*\mathcal{M}$ with $T_z\mathcal{M}$, and because of nondegeneracy its inverse, the cosymplectic form, provides the map $J_c: T_z^*\mathcal{M} \rightarrow T_z\mathcal{M}$. Thus, for a Hamiltonian $H: \mathcal{M} \rightarrow \mathbb{R}$ we have the Hamiltonian system of ordinary differential equations $\dot{z} = J_c dH$, which in canonical coordinates has the familiar form

$$\dot{q}^i = \partial H / \partial p_i, \quad \dot{p}_i = -\partial H / \partial q^i \quad [1]$$

with $i = 1, 2, \dots, N$, where N is the number of degrees of freedom.

Hamilton's equations can also be written in terms of the Poisson bracket $[f, g] := \omega_c(J_c df, J_c dg)$, where $f, g: \mathcal{M} \rightarrow \mathbb{R}$ are smooth phase-space functions. In terms of $z = (q, p)$, Hamilton's equations are

$$\dot{z}^\alpha = J_c^{\alpha\beta} \frac{\partial H}{\partial z^\beta} = [z^\alpha, H] \quad [2]$$

where the Poisson bracket is

$$[f, g] = \frac{\partial f}{\partial z^\alpha} J_c^{\alpha\beta} \frac{\partial g}{\partial z^\beta} \quad [3]$$

with

$$(J_c^{\alpha\beta}) = \begin{pmatrix} 0_N & I_N \\ -I_N & 0_N \end{pmatrix} \quad [4]$$

Note, repeated indices are to be summed with $\alpha, \beta = 1, 2, \dots, 2N$. In [4], 0_N is an $N \times N$ matrix of zeros and I_N is the $N \times N$ unit matrix.

Noncanonical Poisson Brackets

The canonical Poisson bracket description of [2]–[4] suggests a generalization, with antecedents to S Lie and others, that was termed noncanonical Hamiltonian form in the fluid mechanics context by P Morrison and J Greene (1980):

A system has noncanonical Hamiltonian form if it can be written as $\dot{z} = [z, H]$, where the noncanonical Poisson bracket $[,]$ is a Lie product for a realization of a Lie enveloping algebra on phase-space functions.

Recall a Lie enveloping algebra \mathfrak{a} is a Lie algebra, with the usual product $[,]$ that is bilinear, anti-symmetric, and satisfies the Jacobi identity, which in addition has a product $\mathfrak{a} \times \mathfrak{a} \rightarrow \mathfrak{a}$ that satisfies the Leibniz identity $[fg, h] = f[g, h] + [f, h]g$ for all $f, g, h \in \mathfrak{a}$.

The geometric description of noncanonical Hamiltonian form has evolved into a structure called the Poisson manifold, a differential manifold \mathcal{Z} endowed with the binary bracket operation $[,]$ defined on smooth functions, say, $f, g: \mathcal{Z} \rightarrow \mathbb{R}$. Poisson manifolds differ from symplectic manifolds

because the nondegeneracy condition is removed. In coordinates, $[,]$ is given by

$$[f, g] = \frac{\partial f}{\partial z^\alpha} J^{\alpha\beta} \frac{\partial g}{\partial z^\beta}, \quad [5]$$

$$\alpha, \beta = 1, 2, \dots, M$$

where $M = \dim \mathcal{Z}$. Note that J need not have the form of [3], may depend upon the coordinate z , and may have vanishing determinant. Bilinearity, $[f, g] = -[g, f]$ for all f, g , and the Jacobi identity, $[f, [g, h]] + [g, [h, f]] + [h, [f, g]] \equiv 0$, for all f, g, h , imply that the cosymplectic matrix satisfies $J^{\alpha\beta} = -J^{\beta\alpha}$ and

$$J^{\alpha\delta} \frac{\partial J^{\beta\gamma}}{\partial z^\delta} + J^{\beta\delta} \frac{\partial J^{\gamma\alpha}}{\partial z^\delta} + J^{\gamma\delta} \frac{\partial J^{\alpha\beta}}{\partial z^\delta} \equiv 0 \quad [6]$$

respectively, for $\alpha, \beta, \gamma, \delta = 1, 2, \dots, M$.

The local structure of \mathcal{Z} is elucidated by the Darboux-Lie theorem, which states that in a neighborhood of a point $z \in \mathcal{Z}$, for which $\text{rank } J = M$, there exist coordinates in which J has the following form:

$$(J) = \begin{pmatrix} 0_N & I_N & 0 \\ -I_N & 0_N & 0 \\ 0 & 0 & 0_{M-2N} \end{pmatrix} \quad [7]$$

From [7] it is clear that in the right coordinates, the system looks like a canonical N -degree-of-freedom Hamiltonian system with some extraneous coordinates, $M - 2N$ in fact. Through any point of the M -dimensional phase space \mathcal{Z} , there exists a local foliation by symplectic leaves of dimension $2N$.

A consequence of the degeneracy is that there exists a special class of invariants called Casimir invariants that is built into the phase space. Since the rank of J is $2N$, there exist possibly $M - 2N$ independent null eigenvectors. A consequence of the Darboux-Lie theorem is that the independent null eigenvectors exist and, moreover, the null space can in fact be spanned by the gradients of the Casimir invariants, which satisfy $J^{\alpha\beta} \partial C^{(a)} / \partial z^\beta = 0$, where $a = 1, 2, 3, \dots, M - 2N$. That the Casimir invariants are constants of motion follows from

$$\dot{C}^{(a)} = \frac{\partial C^{(a)}}{\partial z^\alpha} J^{\alpha\beta} \frac{\partial H}{\partial z^\beta} = 0 \quad [8]$$

Thus, Casimir invariants are constants of motion for any Hamiltonian. The symplectic leaves of dimension $2N$ are the intersections of the $M - 2N$ surfaces defined by $C^{(a)} = \text{constant}$. Dynamics generated by any H that begins on a particular symplectic leaf remains there. The structure of Poisson manifolds has now been widely studied, but we will not pursue this further here.

Let us turn to infinite-dimensional systems, field theories such as those that govern ideal fluids, where

the governing equations are partial differential equations. Although the level of rigor does not match that achieved for the finite systems described above, formally one can parody most of the steps and, consequently, the finite theory provides cogent imagery and serves as a beacon for shedding light. In infinite dimensions, an analog of [5] is given by

$$\{F, G\} = \int_{\Omega} d\mu \frac{\delta F}{\delta \psi^i} \mathcal{J}^{ij} \frac{\delta G}{\delta \psi^j} =: \left\langle \frac{\delta F}{\delta \psi}, \mathcal{J} \frac{\delta G}{\delta \psi} \right\rangle \quad [9]$$

where F and G are functionals of the functions $\psi^i(\mu, t)$, which are functions of $\mu = (\mu_1, \dots, \mu_n)$, independent variables of some kind, $\delta F / \delta \psi^i$ denotes the functional (variational) derivative, and \langle , \rangle is a pairing between a vector (function) space and its dual. The $\psi^i, i = 1, \dots, n$, are n field components, and now \mathcal{J} is a cosymplectic operator. To be noncanonically Hamiltonian requires antisymmetry, $\{F, G\} = -\{G, F\}$, and the Jacobi identity, $\{F, \{G, H\}\} + \{G, \{H, F\}\} + \{H, \{F, G\}\} \equiv 0$, for all functionals F, G , and H . Antisymmetry requires \mathcal{J} to be skew-symmetric, that is, $\langle f, \mathcal{J}g \rangle = \langle \mathcal{J}^\dagger f, g \rangle = -\langle g, \mathcal{J}f \rangle$. The Jacobi identity for infinite-dimensional systems has a condition analogous to [6]; it can be shown that one need only consider variations of \mathcal{J} when calculating, for example, $\{F, \{G, H\}\}$.

Lie-Poisson Brackets

As noted in the Introduction, the usual variables of fluid mechanics are not a set of canonical variables, and, consequently, the Hamiltonian description in terms of these variables is noncanonical. There is a special general form that the Poisson bracket takes for equations that describe media in terms of Eulerian-like variables, the so-called Lie-Poisson brackets, a special form of noncanonical Poisson bracket. Lie-Poisson brackets describe essentially every fundamental equation that describes classical media. In addition to the equations for the ideal fluid, they describe Liouville's equation for the dynamics of the phase-space density of a collection of particles, the various hierarchy of kinetic theory, the Vlasov equation of plasma physics, and various approximations thereof, and magnetized and other more complicated fluids.

Both finite- and infinite-dimensional Lie-Poisson brackets are intimately associated with a Lie group \mathcal{G} . We use the pairing between a vector space and its dual, \langle , \rangle , where the second slot is reserved for elements of the Lie algebra \mathfrak{g} of \mathcal{G} and the first slot for elements of its dual \mathfrak{g}^* . Thus, $\langle , \rangle : \mathfrak{g}^* \times \mathfrak{g} \rightarrow \mathbb{R}$. In terms of the pairing, noncanonical Lie-Poisson brackets have the following compact form:

$$\{F, G\} = \langle \chi, [F_\chi, G_\chi] \rangle \quad [10]$$

where we suppose the dynamical variable $\chi \in \mathfrak{g}^*$, $[\cdot, \cdot]$ is the Lie algebra product, which takes $\mathfrak{g} \times \mathfrak{g} \rightarrow \mathfrak{g}$, and we have introduced the shorthand $F_\chi := \delta F / \delta \chi$. The quantities F_χ and G_χ are, of course, in \mathfrak{g} . We refer to $\{, \}$ as the “outer” bracket of the realization enveloping algebra and $[\cdot, \cdot]$ as the “inner” bracket of the Lie algebra \mathfrak{g} . The binary operator $[\cdot, \cdot]^\dagger$ is defined as follows:

$$\langle \chi, [f, g] \rangle =: \langle [\chi, g]^\dagger, f \rangle \quad [11]$$

where evidently $\chi \in \mathfrak{g}^*$, $g, f \in \mathfrak{g}$, and $[\cdot, \cdot]^\dagger : \mathfrak{g}^* \times \mathfrak{g} \rightarrow \mathfrak{g}^*$. The operator $[\cdot, \cdot]^\dagger$, which defines the coadjoint orbit, is necessary for obtaining the equations of motion from a Lie–Poisson bracket.

For finite-dimensional systems, the group \mathcal{G} must be a finite-parameter Lie group, the variable ψ corresponds to w , and the cosymplectic form in coordinates is given by $J_{ab} = c_{ab}^c w_c$, where the c_{ab}^c are the structure constants for the Lie algebra \mathfrak{g} , which satisfy

$$\begin{aligned} c_{ab}^c &= -c_{ba}^c \\ c_{ab}^e c_{ec}^d + c_{bc}^e c_{ea}^d + c_{ca}^e c_{eb}^d &= 0 \end{aligned} \quad [12]$$

relations that imply [10] satisfies the antisymmetry condition and the Jacobi identity.

For infinite-dimensional systems, the group \mathcal{G} must be an infinite-parameter Lie group and the cosymplectic operator has the form $\mathcal{J}_{ij} = C_{ij}^k \chi_k$, where C_{ij}^k are structure operators. The meaning of these structure operators will be clarified when we consider brackets for fluid mechanics.

The Fluid State

Fluid mechanics has a long history, and thus it comes as no surprise that the fluid state has been described in many ways. Because the Hamiltonian structure depends on the state variables, some of these ways are described below, beginning with Lagrangian variable description.

Lagrangian Variables

The description of a fluid that is most like that of particle mechanics occurs in terms of variables usually referred to as Lagrangian variables. This description dates to the eighteenth century. The idea behind the use of these variables is a simple one: if a fluid is described as a continuum collection of fluid particles, also called fluid parcels or elements, then its motion is governed by an equation that is an infinite-dimensional version of Newton’s second law and, consequently, as we will see, both the Hamiltonian and the Lagrangian descriptions are infinite degree-of-freedom generalizations of those of ordinary particle mechanics.

The position of a fluid element, referred to a fixed rectangular coordinate systems, is given by $q = q(a, t)$, where $q = (q_1, q_2, q_3)$ and $a = (a_1, a_2, a_3)$ is a continuum label that replaces the index i of [1]. In practice, the label can be any quantity that identifies a fluid particle, but it is often taken to be the position of the fluid particle at time $t=0$ in rectangular coordinates. The quantities $q^i(a, t)$ are coordinates for the configuration space \mathcal{Q} , which is in fact a function space because in addition to the three indices “ i ” there is the continuum label a . We assume that a varies over a fixed domain, $\Omega \subset \mathbb{R}^3$, which is completely filled with fluid, and that the function $q : \Omega \rightarrow \Omega$ is one-to-one and onto. We will assume that as many derivatives of q with respect to a as needed exist, but we will not say more about \mathcal{Q} ; in fact, not much is known about the solution function space for the 3D fluid equations in Lagrangian variables. Often in the Hamiltonian context the functions $q = q(a, t)$ are assumed to be diffeomorphisms and their collection is referred to as the diffeomorphism group.

In the sequel several manipulations are needed and so we record here some identities for later use. Viewing the map $a \mapsto q$ at fixed t as a coordinate change, the Jacobian matrix $\partial q^k / \partial a^i =: q_{,i}^k$ has an inverse given by

$$\frac{\partial q^k}{\partial a^i} \frac{A_i^k}{\mathfrak{J}} = \delta_i^j \quad [13]$$

where A_i^k is the cofactor of $q_{,i}^k$ and \mathfrak{J} is its determinant. A convenient expression for A_i^k is given by

$$A_i^k = \frac{1}{2} \epsilon_{kjl} \epsilon^{imn} \frac{\partial q^j}{\partial a^m} \frac{\partial q^l}{\partial a^n} \quad [14]$$

where $\epsilon_{ijk} (= \epsilon^{ijk})$ is the skew-symmetric tensor (density). Evidently, $\partial \mathfrak{J} / \partial q_{,i}^j = A_i^j$ follows from [13].

Eulerian Variables

In the Lagrangian variable description, one picks out a particular particle, labeled by a , and keeps track in time t of where it goes. However, in the Eulerian variable description, one stays at a spatial observation point $r = (x_1, x_2, x_3) \in \Omega$ and monitors the nature of the fluid at r at time t .

The most important Eulerian variable is the Eulerian velocity field $v(r, t)$. This quantity is the velocity of the particular fluid element that is located at the spatial point r at time t . The label of that particular fluid element is given by $a = q^{-1}(r, t)$, and so

$$v(r, t) = \dot{q}(a, t)|_{a=q^{-1}(r, t)} := \dot{q} \circ q^{-1}(r, t) \quad [15]$$

where $\dot{\cdot}$ denotes differentiation with respect to time at fixed label a . Attached to a fluid element is a certain amount of mass described by a density

function $\rho_0(a)$. As the fluid moves so that $a \mapsto q$, the volume of an infinitesimal region will change, but its mass must remain fixed. The statement of local mass conservation is $\rho d^3r = \rho_0 d^3a$, where d^3a is an initial infinitesimal volume element that maps to d^3q at time t , and $d^3r = \mathfrak{J} d^3a$. (When integrating over Ω we will replace d^3q by d^3r .) Thus, we obtain

$$\rho(r, t) = \frac{\rho_0(a)}{\mathfrak{J}(a, t)} \Big|_{a=q^{-1}(r, t)} = \frac{\rho_0}{\mathfrak{J}} \circ q^{-1}(r, t) \quad [16]$$

where recall the Jacobian $\mathfrak{J} = \det(q^i, j)$. Besides the density, for the ideal fluid, one attaches an entropy per unit mass, $s = s_0(a)$, to a fluid element, and this quantity remains fixed in time. In the Eulerian description this gives rise to the entropy field

$$s(r, t) = s_0(a) \Big|_{a=q^{-1}(r, t)} = s_0 \circ q^{-1}(r, t) \quad [17]$$

One could attach other scalar, vector, etc., quantities to the fluid element, but we will not pursue this. In the usual ideal fluid closure only the above variables are considered.

Equations [15]–[17] express the Euler–Lagrange map. There is a natural representation of this map in terms of the Eulerian density variables, $M := \rho v$, ρ , and $\sigma := \rho s$, the momentum, mass, and entropy densities, respectively, which, as will be seen, are variables in which the noncanonical Poisson bracket has Lie–Poisson form.

Other Variables

Fluid mechanics is rife with variables that have been used for its description. For example, Euler, Monge, Clebsch, and others introduced potential representations, of varying generality, for the Eulerian velocity field, an example being

$$v(r, t) = \alpha \nabla \beta + \nabla \phi \quad [18]$$

where the three components of v are replaced by the functions α , β , and ϕ , all of which depend on (r, t) .

Often reduced variables that are tailored to specific ideal flows with less generality than those described by ρ , s , and v are considered. Examples include incompressible flow with $\nabla \cdot v = 0$, vortex dynamics, including contour dynamics and point vortex dynamics, flow governed by the shallow-water equations, quasigeostrophy, etc. The Hamiltonian structure in terms of these reduced variables derives from that of the parent model in terms of Lagrangian variables. Specific variables may embody constraints, and understanding these constraints, although tractable, can be a cause of confusion. Pursuing this further is beyond the scope here.

Hamilton's Principle for Fluid

Lagrange, in his famous work of 1788, *Mécanique Analytique*, produced in essence a variational principle for incompressible fluid flow in terms of Lagrangian variables. The generalization to compressible flow awaited the discovery of thermodynamics, and that is what we describe here. In traditional mechanics nomenclature, this variational principle is an infinite-dimensional generalization of what is known variously as the action principle, the principle of least action, or Hamilton's principle, whereby one constructs, on physical grounds, a Lagrangian function on TQ used in the action principle, where Q is the function space of the $q(a, t)$.

Construction of the Lagrangian requires identification of the potential energy, and this requires thermodynamics, because potential energy is stored in terms of pressure and temperature. A basic assumption of the fluid approximation is that of local thermodynamic equilibrium. In the energy representation of thermodynamics, the extensive energy is treated as a function of the entropy and the volume. For a fluid, it is convenient to consider the energy per unit mass, denoted by U , to be a function of the entropy per unit mass, s , and the mass density, ρ , a measure of the volume. The intensive quantities, pressure and temperature, are given by $T = \partial U / \partial s$ and $p = \rho^2 \partial U / \partial \rho$. Choices for U produce equations of state. For barotropic or isentropic flow, U depends only on ρ . For an ideal monatomic gas $U(\rho, s) = c \rho^{\gamma-1} \exp(\alpha s)$, where c , γ , and α are constants. The function U could also depend on additional scalar quantities, such as a quantity known as spice that has been considered in oceanography.

Conventional thermodynamic variables can be viewed as Eulerian variables with a static velocity field. Thus, we write $U(\rho, s)$, where ρ and s are spatially independent or, if the system has only locally relaxed, these variables can be functions of r . For the ideal fluid, each fluid element can be viewed as a self-contained isentropic thermodynamic system that moves with the fluid. Thus, the total fluid potential energy functional is given by $V[q] = \int_{\Omega} d^3a \rho_0 U(s_0, \rho_0 / \mathfrak{J})$, which is a functional of q that depends only upon \mathfrak{J} and hence only upon $\partial q / \partial a$.

The next item required for constructing Hamilton's principle is the kinetic energy functional, which is given by $T[q, \dot{q}] = \int_{\Omega} d^3a \rho_0 \dot{q}^2 / 2$, where $\dot{q}^2 := \eta_{ij} \dot{q}^i \dot{q}^j$, with the Cartesian metric $\eta_{ij} := \delta_{ij}$. This metric and its inverse can be used to raise and lower indices.

The Lagrangian functional is $L[q, \dot{q}] := T - V$, where $L[q, \dot{q}] = \int_{\Omega} d^3a \mathcal{L}(q, \dot{q}, \partial q / \partial a)$ and \mathcal{L} is the

Lagrangian density, in terms of which the action functional of Hamilton's principle is given by

$$S[q] = \int_{t_0}^{t_1} dt L[q, \dot{q}] = \int_{t_0}^{t_1} dt \int_{\Omega} d^3a \left[\frac{1}{2} \rho_0 \dot{q}^2 - \rho_0 U \right] \quad [19]$$

The end conditions for Hamilton's principle for the fluid are the same as those of mechanics, that is, $\delta q(a, t_0) = \delta q(a, t_1) = 0$. The nonpenetration condition, $\delta q \cdot \hat{n} = 0$ on $\partial\Omega$, where \hat{n} is a unit normal vector is also assumed. Other boundary conditions, such as periodic and free boundary conditions, are also possibilities. Hamilton's principle amounts to $\delta S / \delta q(a, t) = 0$, which, with the end and boundary conditions, implies the following equations of motion:

$$\rho_0 \ddot{q}_i + A_i^j \frac{\partial}{\partial a^j} \left(\frac{\rho_0^2}{\mathcal{J}^2} \frac{\partial U}{\partial \rho} \right) = 0 \quad [20]$$

Here we have used $\partial A_i^j / \partial a^j = 0$, which can be seen using [14]. Equation [20] amounts to Newton's second law for the ideal fluid, which is made clearer by using the following useful identity:

$$\frac{\partial}{\partial q^k} = \frac{1}{\mathcal{J}} A_k^i \frac{\partial}{\partial a^i} \quad [21]$$

Alternatively, upon using [13], [20] is sometimes written in the form

$$\rho_0 \ddot{q}_i \frac{\partial q^i}{\partial a^i} + \mathcal{J} \frac{\partial}{\partial a^i} \left(\frac{\rho_0^2}{\mathcal{J}^2} \frac{\partial U}{\partial \rho} \right) = 0 \quad [22]$$

The Eulerian variable force law follows from [20] upon using [21]:

$$\rho \left(\frac{\partial v}{\partial t} + v \cdot \nabla v \right) = -\nabla p \quad [23]$$

where $v = v(r, t)$. The remaining Eulerian equations of mass conservation and entropy advection follow from the constraints that s_0 and ρ_0 are constant on fluid elements. Time differentiation and the transformations of [16] and [17] yield

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0 \quad [24]$$

$$\frac{\partial s}{\partial t} + v \cdot \nabla s = 0 \quad [25]$$

Equations [23]–[25] together with a given function $U(\rho, s)$ and the relation $p = \rho^2 \partial U / \partial \rho$ constitute the Eulerian description.

Variational principles similar to that described above exist for essentially all ideal fluid models, including incompressible flow, magnetohydrodynamics, the two-fluid equations of plasma physics, etc.

Eulerian Action Principles

Some early researchers sought variational principles that directly produce the ideal fluid equations in Eulerian form. Because the Eulerian form of the equations does not treat the fluid as a collection of particles, the resulting action principles possess a certain awkwardness. Below, we describe three approaches to such action principles.

Clebsch action The action principle for electromagnetism proceeds by introducing the 4-vector potential. In a similar way, the Clebsch action principle anticipates this idea by using a potential representation of the velocity field, an example being that of [18].

Although compressible flow with an arbitrary equation of state can be treated in full generality, for simplicity and variety we will restrict to incompressible flow and set $\nabla \cdot v \equiv 0$. This constraint is enforced by requiring ϕ to be dependent on α and β according to $\phi[\alpha, \beta] := -\Delta^{-1}(\alpha \nabla \beta)$, where Δ^{-1} is the inverse Laplacian. The Clebsch action is then written as follows:

$$S_C[\alpha, \beta] := \int_{t_0}^{t_1} dt \int_{\Omega} d^3r \left[\beta \alpha_t - \frac{1}{2} v^2 \right] \quad [26]$$

where the subscript t denotes differentiation at fixed r , we have set $\rho \equiv 1$, and v is a shorthand for the expression of [18] with $\phi = \phi[\alpha, \beta]$. The form of S_C is that of the phase-space action that produces Hamilton's equations upon independent variation of the configuration space coordinate and its conjugate momentum, which are here α and β , respectively. Thus, we require $\delta \alpha(r, t_0) = \delta \alpha(r, t_1) = 0$, but no condition is needed for $\delta \beta$ at $t_{0,1}$. We also require $\hat{n} \cdot v = 0$ on $\partial\Omega$. The variations $\delta S_C / \delta \beta = 0$ and $\delta S_C / \delta \alpha = 0$ imply

$$\begin{aligned} \alpha_t &= \frac{\delta H}{\delta \beta} = -v \cdot \nabla \alpha \\ \beta_t &= -\frac{\delta H}{\delta \alpha} = -v \cdot \nabla \beta = 0 \end{aligned} \quad [27]$$

an infinite-dimensional version of [1] with $H := \int_{\Omega} d^3r v^2 / 2$. Evidently, both α and β are advected by the flow.

Because the vorticity, $\zeta := \nabla \times v = \nabla \alpha \times \nabla \beta$, knowledge of α and β determines ζ and one can invert the curl operator to obtain v in the usual way. The intersection of level sets of α and β define vortex lines, and, evidently, these quantities, like the entropy for compressible dynamics, are constant on fluid elements. It is not difficult to show that the advection of α and β implies the correct dynamical equation for incompressible v .

Herivel–Lin action The Herivel–Lin action incorporates [24] and [25] as constraints with Lagrange

multipliers, φ and $\rho\beta$. (Here β is not the Clebsch β and the factor of ρ is included for convenience.) It was discovered early on that these constraints were not enough to achieve complete generality and so a new one, known as the Lin constraint, was added. The Lin constraint corresponds to constancy of the fluid particle label. One defines an Eulerian label field by setting $q(a, t) = r$ and solving for the label $a = q^{-1}(r, t) =: a(r, t)$. Conservation of particle identity is thus given by $a_t + v \cdot \nabla a = 0$, and this constraint is associated with a Lagrange multiplier $\gamma = (\gamma_1, \gamma_2, \gamma_3)$. The Herivel–Lin action is thus given by

$$S_{\text{HL}}[v, \rho, s, a; \varphi, \beta, \gamma] = \int_{t_0}^{t_1} dt \int_{\Omega} d^3r \left(\frac{1}{2} \rho v^2 - \rho U(\rho, s) + \varphi[\rho_t + \nabla \cdot (\rho v)] - \rho\beta[s_t + v \cdot \nabla s] - \rho\gamma \cdot [a_t + v \cdot \nabla a] \right) \quad [28]$$

Variation of [28] with respect to the Lagrange multipliers just reproduces the constraints; however, variation with respect to v , ρ , s , and a produces equations that imply [23]. Moreover, every flow can be shown to be an extremal of S_{HL} .

Euler–Poincaré–Hamel action Another approach is to use directly constrained variations. The essential idea is to only consider Eulerian variable variations that are induced by underlying Lagrangian variable variations δq , the so-called dynamically accessible variations. Explicitly, a basic Eulerian variation $\eta = (\eta_1, \eta_2, \eta_3)$ is given by $\eta(r, t) = \delta q(a, t)|_{a=q^{-1}(r, t)}$. In terms of this quantity, the dynamically accessible variations of the Eulerian velocity field, density, and entropy are given, respectively, by $\delta v = \eta_t + v \cdot \nabla \eta - \eta \cdot \nabla v$, $\delta \rho = -\nabla \cdot (\rho \eta)$, and $\delta s = -\eta \cdot \nabla s$. Upon inserting them into the variation of

$$S_{\text{EPH}}[\eta] = \int_{t_0}^{t_1} dt \int_{\Omega} d^3r \left[\frac{1}{2} \rho v^2 - \rho U(\rho, s) \right] \quad [29]$$

and integrating by parts gives

$$\delta S_{\text{EPH}} = \int_{t_0}^{t_1} dt \int_{\Omega} d^3r [\dots] \cdot \eta = 0$$

where $[\dots]$ is equivalent to [23]. Thus, assuming η is arbitrary, we obtain directly the equation of motion.

There is a version of this kind of constrained variational principle for all ideal fluid and plasma equations. Also, it possesses a geometric interpretation. In a more practical vein, constrained variations can be used to derive reduced models, and dynamically accessible variations can also be used for stability calculations. Exploring these ideas is outside the present scope.

Fluid Hamiltonian Description

Having described variational principles, we turn to the associated canonical and noncanonical Hamiltonian descriptions.

Canonical Description

Because the action of [19] is of standard form, it is convex in \dot{q} and the Legendre transform follows easily: the canonical momentum density is $\pi_i(a, t) := \delta L / \delta \dot{q}^i(a) = \rho_0 \dot{q}_i$ and $H[q, \pi] = \int_{\Omega} d^3a [\pi \cdot \dot{q} - \mathcal{L}] = \int_{\Omega} d^3a [\pi^2 / (2\rho_0) + \rho_0 U]$. Hamilton's equations are then

$$\dot{q}^i = \frac{\delta H}{\delta \pi_i} = \{q^i, H\}, \quad \dot{\pi}_i = -\frac{\delta H}{\delta q^i} = \{\pi_i, H\} \quad [30]$$

an infinite-dimensional version of [1], with the canonical Poisson bracket

$$\{F, G\} = \int_{\Omega} d^3a \left[\frac{\delta F}{\delta q} \cdot \frac{\delta G}{\delta \pi} - \frac{\delta G}{\delta q} \cdot \frac{\delta F}{\delta \pi} \right] \quad [31]$$

(Note, $\delta q^i(a) / \delta q^j(a') = \delta^i_j \delta(a - a')$, a relation analogous to $\partial q^i / \partial q^j = \delta^i_j$ for finite systems.)

Reduction to Noncanonical Poisson Brackets

Reduction is a procedure for reducing the size of a Hamiltonian system. Given constants of motion in involution, that is, with pairwise vanishing Poisson brackets, the dimension of a Hamiltonian system can be reduced by 2 for each such constant of motion. However, when constants do not commute, the situation is more complicated and one must invoke a theory due to Lie, Poincaré, Cartan, and others. Associated with invariants are symmetries, and so a complete discussion of this theory requires examination of symmetry groups and associated geometry. For the ideal fluid, the map from the Lagrangian to the Eulerian descriptions is an example of reduction, whereby the Poisson bracket of [31] is mapped into a noncanonical Poisson bracket. En route to describing this example, a brief discussion of reduction of finite systems is considered first.

Reduction of Finite-Dimensional Systems

Consider a canonical system with the phase space \mathcal{M} , a $2N$ -dimensional symplectic manifold. In a coordinate patch with coordinates $z = (q, p)$ the system has the canonical description of [2]–[4]. Suppose we have a map $P: \mathcal{M} \rightarrow \mathfrak{m}^*$, where \mathfrak{m}^* is some $M < 2N$ -dimensional space described by coordinates $w = (w_1, w_2, \dots, w_M)$. In coordinates, this map is represented in terms of functions $w_a = w_a(z)$,

with $a=1,2,\dots,M$, which, because $M < 2N$, is always noninvertible. Suppose $f, g: \mathcal{M} \rightarrow \mathbb{R}$ obtain their z -dependence through the functions w , that is, $f(z) = \bar{f}(w(z)) = \bar{f} \circ w$. Making use of the chain rule yields

$$[f, g] = \frac{\partial \bar{f}}{\partial w_a} J_{ab} \frac{\partial \bar{g}}{\partial w_b} \quad [32]$$

where the quantity

$$J_{ab} := \frac{\partial w_a}{\partial z^\alpha} J_c^{\alpha\beta} \frac{\partial w_b}{\partial z^\beta} \quad [33]$$

is in general a function of z . However, it is possible that J_{ab} may only depend on w . When this happens, we have a reduction of the phase space \mathcal{M} .

If the original dynamics of interest has the Hamiltonian vector field generated by $H(z)$, and if it is possible that $H(z)$ can be expressed solely in terms of the w 's, that is, $H(z) = \bar{H}(w)$, then the system has been reduced. Clearly, this is a statement of symmetry, since the function $H(z)$ in reality depends on a fewer number of variables, the w 's.

A beautiful form of reduction occurs when the map P has a special form $w_a = L_a^i(q)p_i$, where the quantity L is associated with a symmetry group. An identity for what is required of L_a^i in order for the transformed bracket to be expressible in terms of the w 's can be worked out, but this is explained in terms of Lie groups. If the space \mathfrak{m} is a Lie algebra \mathfrak{g} , then the functions \bar{f}, \bar{g} are real-valued functions on \mathfrak{g}^* that can be extended by left or right translation to functions \bar{f}, \bar{g} on $T^*\mathfrak{G}$. Thus, \bar{f} restricted to $T^*\mathfrak{G}$ at the identity, $T_e^*\mathfrak{G} = \mathfrak{g}^*$, is \bar{f} . Because $T^*\mathfrak{G}$ is a cotangent bundle, it carries the canonical Poisson bracket and we get a natural map P , called a momentum map, into the dual of a Lie algebra. This geometrical description of obtaining brackets on \mathfrak{g}^* from brackets on $T^*\mathfrak{G}$ is a case of Marsden–Weinstein reduction. In the early 1980s, these authors and others developed the geometrical interpretation of the noncanonical Poisson brackets for the ideal fluid.

Ideal Fluid Noncanonical Poisson Brackets

The Euler–Lagrange map of the fluid is of the form of the map P above. It maps the canonical bracket of [31] into a noncanonical Poisson bracket. If we use the Eulerian variables $M := \rho v$, ρ , and $\sigma := \rho s$, then the resulting noncanonical bracket is of Lie–Poisson form. To effect this map, one must vary [15]–[17] to relate functional derivatives with respect to q and π to those with respect to M, ρ , and σ . This amounts to working out the chain rule for functionals. Upon

doing this, one obtains the following noncanonical bracket:

$$\begin{aligned} \{F, G\} = & - \int_{\Omega} \left[M_i \left(\frac{\delta F}{\delta M_j} \frac{\partial}{\partial x^j} \frac{\delta G}{\delta M_i} - \frac{\delta G}{\delta M_j} \frac{\partial}{\partial x^j} \frac{\delta F}{\delta M_i} \right) \right. \\ & + \rho \left(\frac{\delta F}{\delta M} \cdot \nabla \frac{\delta G}{\delta \rho} - \frac{\delta G}{\delta M} \cdot \nabla \frac{\delta F}{\delta \rho} \right) \\ & \left. + \sigma \left(\frac{\delta F}{\delta M} \cdot \nabla \frac{\delta G}{\delta \sigma} - \frac{\delta G}{\delta M} \cdot \nabla \frac{\delta F}{\delta \sigma} \right) \right] d^3 r \quad [34] \end{aligned}$$

This bracket, together with the Hamiltonian $\bar{H}[M, \rho, \sigma] = \int_{\Omega} d^3 r [M^2/(2\rho) + \rho U(\rho, \sigma/\rho)]$ generates the ideal fluid equations. This Hamiltonian follows from $\bar{H}[M, \rho, \sigma] := H[q, \pi]$ with $H[q, \pi] = \int_{\Omega} d^3 a [\pi^2/(2\rho_0) + \rho_0 U]$. The bracket of [34] is clearly seen to be linear in the variables M, ρ , and σ , and the form of the cosymplectic operator and structure operators C_{ij}^k can be obtained by integration by parts. The Lie group in this case can be seen to be an extension by semidirect product of the diffeomorphism group.

An alternative form of the noncanonical Poisson bracket is given in terms of the variables v, ρ , and s . Upon changing to these coordinates, the noncanonical Poisson bracket transforms into

$$\begin{aligned} \{F, G\} = & - \int_{\Omega} \left[\left(\frac{\delta F}{\delta \rho} \nabla \cdot \frac{\delta G}{\delta v} - \frac{\delta G}{\delta \rho} \nabla \cdot \frac{\delta F}{\delta v} \right) \right. \\ & + \left(\frac{\nabla \times v}{\rho} \cdot \frac{\delta G}{\delta v} \times \frac{\delta F}{\delta v} \right) \\ & \left. + \frac{\nabla s}{\rho} \cdot \left(\frac{\delta F}{\delta s} \frac{\delta G}{\delta v} - \frac{\delta G}{\delta s} \frac{\delta F}{\delta v} \right) \right] d^3 r \quad [35] \end{aligned}$$

which, with the Hamiltonian $H[v, \rho, s] = \int_{\Omega} d^3 r [\rho v^2/2 + \rho U(\rho, s)]$, produces the Eulerian fluid equations of [23]–[25] directly as $v_t = \{v, H\}$, $\rho_t = \{\rho, H\}$, and $s_t = \{s, H\}$, respectively. Observe that in these variables, the bracket is no longer of Lie–Poisson form.

Conclusion

In a general sense, Hamiltonian dynamics is about coordinate changes, and it is clear from the above that there is no shortage of coordinates for describing the ideal fluid. The most intuitive form of fluid equations (at present) is the Eulerian form, and this possesses a noncanonical Hamiltonian description. Other noncanonical variables are also used for both less and more general fluid systems than those described above. Vortex dynamics, shallow-water theory, and other equations of geophysical fluid dynamics are possibilities, as well as equations from plasma physics and other disciplines. The general story for these systems is much the same as above, although in some descriptions constraints are involved and they can complicate matters.

There are various motivations for pursuing an understanding of the Hamiltonian structure of fluids, but ultimately these motivations are the same as those for investigating the Hamiltonian dynamics of particle and other finite degree-of-freedom systems. Hamiltonian theory serves as an organizing framework, one that can be used for the derivation and approximation of systems. If one understands something about a particular Hamiltonian system, then often it can be said to be true of a general class of Hamiltonian systems. By now, many applications have been worked out, some of which can be accessed from the literature cited below.

See also: Adiabatic Piston; Adiabatic Piston; Bi-Hamiltonian Methods in Soliton Theory; Bi-Hamiltonian Methods in Soliton Theory; Classical r -Matrices, Lie Bialgebras, and Poisson Lie Groups; Contact Manifolds; Contact Manifolds; Hamiltonian Group Actions; Infinite-Dimensional Hamiltonian Systems; Korteweg–de Vries Equation and other Modulation Equations; Korteweg–de Vries Equation and Other Modulation Equations; Stochastic Hydrodynamics; Stochastic Hydrodynamics.

Hamiltonian Group Actions

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Introduction

The idea of a Hamiltonian flow on a symplectic manifold has its roots in Hamilton's equations, which govern the trajectory of a particle in phase space (the space parametrizing coordinates and momenta of a classical particle). A fundamental idea in theoretical physics (Noether's theorem) is that to every symmetry in a physical system (such as a group action), there is an associated conserved quantity: invariance under translation corresponds to conservation of linear momentum, invariance under rotation corresponds to conservation of angular momentum and so on, and these momenta are functions on the phase space. The mathematical formulation of this idea is the idea of the moment map associated to a group action on a symplectic manifold; the group action is obtained from the Hamiltonian flow of the moment map.

This article will describe some basic features of moment maps associated to Hamiltonian group

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actions, and some recent results about the geometry and topology of symplectic manifolds which have such group actions. We first define Hamiltonian group actions and list some of their properties. Next we give the definition of the symplectic quotient, which is a means of dividing out the symmetry to form a new symplectic manifold. We also explain some properties of the quotient construction. The convexity theorem and the moment polytope are outlined and toric manifolds (a particular type of symplectic manifold with a Hamiltonian torus action of maximal dimension) are defined. Finally, we list some properties of cohomology rings of symplectic quotients.

Two standard references on this material are the books of Cannas da Silva (2001) and McDuff and Salamon (1995). An authoritative and comprehensive reference is the monograph by Guillemin, Ginzburg and Karshon (2002).

Hamiltonian Group Actions

Let (M, ω) be a symplectic manifold. The Hamiltonian vector field ξ_H generated by a function H is defined by

$$\omega_m(\xi_H, Y) = dH_m(Y)$$

for any $Y \in T_m M$. If $X \in \mathfrak{g} \mapsto X^\#$ are the vector fields on M generated by the symplectic action of a compact Lie group G with Lie algebra \mathfrak{g} , then the moment map $\mu: M \rightarrow \mathfrak{g}^*$ is defined by two properties:

1. $d\mu_m(Y)(X) = \omega_m(X^\#, Y)$ for any $Y \in T_m M$: in other words the function $\mu_X: M \rightarrow \mathbb{R}$ defined by

$$\mu_X(m) \stackrel{\text{def}}{=} \mu(m)(X)$$

is the Hamiltonian function generating the vector field $X^\#$.

2. $\mu: M \rightarrow \mathfrak{g}^*$ is equivariant (where G acts on \mathfrak{g}^* by the coadjoint action).

Remark 1 In this article, we shall only consider actions of compact connected Lie groups, although the definition of Hamiltonian group action may be extended to noncompact groups. In particular, unless otherwise specified the term “torus” refers to the compact torus $T \cong U(1)^n$.

Remark 2 (Existence and uniqueness of moment maps). One sees that $\mathcal{L}_{X^\#}\omega = d(\iota_{X^\#}\omega)$, so that $\iota_{X^\#}\omega$ is closed. The moment map μ_X exists if and only if $\iota_{X^\#}\omega$ is also “exact.” The moment map need not always exist: for example, if S^1 acts on T^2 by

$$e^{iX} : (e^{i\theta_1}, e^{i\theta_2}) \mapsto (e^{i(\theta_1+X)}, e^{i\theta_2})$$

we see that for the standard symplectic form $\omega = d\theta_1 \wedge d\theta_2$ we have $\iota_{X^\#}\omega = d\theta_2$. Since θ_2 is only defined mod 2π we see that the moment map does not exist as a map into \mathbb{R} . Conditions guaranteeing the existence of a moment map (other than M being simply connected) include the hypothesis that G is semisimple (Guillemin and Sternberg (1990, theorem 26.1)); conditions on the existence and uniqueness of the moment map can be formulated in terms of Lie algebra cohomology (see Guillemin and Sternberg (1990)). The obstruction to the existence of the moment map for a symplectic action of G is an element of $H^1(\mathfrak{g})$; the obstruction to uniqueness of the moment map is an element of $H^2(\mathfrak{g})$, where \mathfrak{g} is the Lie algebra of G . See Guillemin and Sternberg (1990, proposition 24.1).

Basic Properties of Moment Maps

Proposition 1 (Guillemin–Sternberg (1982, 1984))

$$\text{Im}(d\mu_m)^\perp = \text{Lie}(\text{Stab}(m))$$

where \perp denotes the annihilator under the canonical pairing $\mathfrak{g}^* \otimes \mathfrak{g} \rightarrow \mathbb{R}$.

Proof We have

$$\omega(Y_m^\#, Z) = d\mu_Y(Z) = \langle Y, d\mu_m(Z) \rangle$$

for all $Z \in T_m M$. Thus, Y annihilates all $\xi \in \text{Im}(d\mu_m)$ if and only if $Y \in \text{Lie}(\text{Stab}(m))$.

Corollary 1 Zero is a regular value of μ if and only if $\text{Stab}(m)$ is finite for all $m \in \mu^{-1}(0)$. In this situation, $\mu^{-1}(0)$ is a manifold and the stabilizer of the action at any point in $\mu^{-1}(0)$ is finite.

Example 1 Let T be a torus acting on M and let $F \subset M^T$ be a component of the fixed-point set. Then for any $f \in F$, we have $d\mu_f = 0$, so $\mu(F)$ is a point.

Proposition 2

- (i) If $H \subset G$ are two groups acting in a Hamiltonian fashion on a symplectic manifold M , then $\mu_H = \pi \circ \mu_G$ where $\pi: \mathfrak{g}^* \rightarrow \mathfrak{h}^*$ is the projection map. In other words, if $X \in \mathfrak{h}$, then $\mu_H(m)(X) = \mu_G(m)(X)$ for any $m \in M$. One example that frequently arises is the case when $H = T$ is a maximal torus of a compact Lie group G .
- (ii) More generally if $f: H \rightarrow G$ is a Lie group homomorphism, and the two groups G and H act in a Hamiltonian fashion on a symplectic manifold M , in such a way that the action is compatible with the homomorphism f , then $\mu_H = f^* \circ \mu_G$ where $f^*: \mathfrak{g}^* \rightarrow \mathfrak{h}^*$ is induced from the homomorphism f . (The case (i) is the special case where f is the inclusion map.)
- (iii) If two symplectic manifolds M_1 and M_2 are acted on in a Hamiltonian fashion by a group G with moment maps μ_1 and μ_2 , then the moment map for the diagonal action of G on $M_1 \times M_2$ with the product symplectic structure is $\mu_1 + \mu_2$.

Example 2 The standard symplectic form on S^2 is $\omega = -d\cos\theta \wedge d\phi = -dz \wedge d\phi$ (where θ is the polar angle, ϕ is the azimuthal angle, and z is the height function). The associated moment map for the action of $U(1)$ on S^2 by rotation about the z axis is $\mu(z, \phi) = z$.

Example 3 If $\mathbb{R}^2 = \mathbb{C}$ has the symplectic structure $\omega = dx \wedge dy$, the moment map for the standard action of $U(1)$ on \mathbb{R}^2 with multiplicity $m \in \mathbb{Z}$, in other words the action

$$u \in U(1) : z \in \mathbb{C} \mapsto u^m z$$

is $\mu(x, y) = -m(x^2 + y^2)/2$.

Example 4 Suppose a torus T acts on \mathbb{C} preserving the standard symplectic structure, and suppose the action factors through a homomorphism $B: T \rightarrow U(1)$ which can be written as

$$B(\exp_T X) = \exp_{U(1)}(\beta(X))$$

in terms of a linear map $\beta \in \mathfrak{t}^*$ that maps the integer lattice of \mathfrak{t} into \mathbb{Z} (in other words, a weight) and the exponential maps

$$\exp_T : \mathfrak{t} \rightarrow T$$

and

$$\exp_{U(1)} : \mathbb{R} \rightarrow U(1)$$

(the latter being normalized as $\exp_{U(1)}(t) = e^{2\pi it}$). Then, by Proposition 2(ii) and Example 3 we see that the moment map for the action of T on \mathbb{C} is

$$\mu(z) = -\frac{1}{2}\beta|z|^2$$

It follows that if T acts on \mathbb{C}^n via a collection of weights $\beta_1, \dots, \beta_n \in \mathfrak{t}^*$, then the moment map is

$$\mu(z_1, \dots, z_n) = -\frac{1}{2} \sum_{j=1}^n |z_j|^2 \beta_j$$

and the image of the moment map is the cone in \mathfrak{t}^* spanned by $\{\beta_1, \dots, \beta_n\}$.

The Symplectic Quotient

Since the moment map μ is equivariant, we may form the symplectic quotient (or Marsden–Weinstein reduction)

$$M_{\text{red}} = M_0 = \mu^{-1}(0)/G$$

The symplectic structure on M descends to give a symplectic structure on M_0 . Corollary 1 implies that if 0 is a regular value of μ , then M_0 is an orbifold.

Remark 3 Another way to formulate Corollary 1 is that if G acts freely, 0 is a regular value of μ so $\mu^{-1}(0)$ is a manifold with a free G action, and hence $\mu^{-1}(0)/G$ is also a manifold. If the G action is only locally free, then $\mu^{-1}(0)$ is still a manifold, but the quotient $\mu^{-1}(0)/G$ is only an orbifold.

Remark 4 The definition of orbifold is due to Satake (1957); an alternate formulation is given in the paper by Henriques and Metzler (2004) and references cited there.

If T is a torus, then the equivariance condition on the moment map reduces to invariance, so we may form the reduced space $M_t = \mu^{-1}(t)/T$ for any regular value $t \in \mathfrak{t}^*$ of the moment map μ ; the space M_t is a symplectic orbifold for any regular value t of μ .

Example 5 Let $U(1)$ act diagonally on \mathbb{C}^n equipped with the standard symplectic structure

$$\begin{aligned} \omega &= \frac{i}{2} \sum_{j=1}^n dz_j \wedge d\bar{z}_j \\ &= \sum_{j=1}^n dx_j \wedge dy_j \end{aligned} \quad [1]$$

where $z_j = x_j + iy_j$. The moment map for this action is

$$\mu(z_1, \dots, z_n) = -\frac{1}{2} \sum_{j=1}^n |z_j|^2$$

so the symplectic quotient $\mu^{-1}(-1/2)/U(1)$ is complex projective space

$$S^{2n-1}/U(1) \cong \mathbb{CP}^{n-1}$$

More generally we may consider the reduced space $M_\lambda = \mu^{-1}(\mathcal{O}_\lambda)/G$ when \mathcal{O}_λ is the orbit in \mathfrak{g}^* through $\lambda \in \mathfrak{g}^*$ (coadjoint orbit). All such orbits may be parametrized by $\lambda \in \mathfrak{t}_+^*$, where \mathfrak{t}_+^* is a chosen positive Weyl chamber in \mathfrak{t}^* .

Example 6 Let $U(n)$ act on \mathbb{C}^n in the standard way, where \mathbb{C}^n is equipped with the standard symplectic structure [1]. The moment map for this action is

$$\mu(z_1, \dots, z_n)_{jk} = \frac{i}{2} z_j \bar{z}_k \quad [2]$$

which is the (j, k) element of a matrix in the Lie algebra of $U(n)$. The standard symplectic form on \mathbb{C}^n descends under reduction to the standard symplectic form on \mathbb{CP}^{n-1} (which corresponds to the Fubini–Study metric).

Example 7 (Coadjoint orbits). Let $\lambda \in \mathfrak{g}^*$. We define a symplectic structure ω_λ on the coadjoint orbit \mathcal{O}_λ (in terms of the vector fields $X^\#, Y^\#$ generated by the action of $X, Y \in \mathfrak{g}$) by $\omega_\lambda(X^\#, Y^\#) = -\lambda([X, Y])$ at the point $\lambda \in \mathcal{O}_\lambda$ (and everywhere else on the orbit by equivariance). The moment map for the action of G on \mathcal{O}_λ with respect to this symplectic structure is the inclusion of \mathcal{O}_λ in \mathfrak{g}^* . (The symplectic structure on the orbit was found by Kirillov and Kostant; see, for instance, Berline *et al.* (1992, section 7.5).

Example 8 (The shifting trick). Define a symplectic structure Ω on $M \times \mathcal{O}_\lambda$ by

$$\Omega = \omega^M - \omega_\lambda$$

Then for the moment map with respect to the induced action of G on $M \times \mathcal{O}_\lambda$ we have

$$M_\lambda \cong (M \times \mathcal{O}_\lambda)_0$$

Corollary 2 *Combining Example 6 with Proposition 2(ii) we see that for any linear action of a group G on $\mathbb{C}P^{n-1}$ (i.e., an action factoring through a representation $G \rightarrow U(n)$, or in other words an action descending from a linear action on \mathbb{C}^n) the moment map factors as*

$$\mu = \pi \circ \hat{\mu}$$

where $\hat{\mu}: \mathbb{C}P^{n-1} \rightarrow \mathfrak{u}(n)^*$ is given in [3] below, and $\pi: \mathfrak{u}(n)^* \rightarrow \mathfrak{g}^*$ is the projection map.

In particular, one often requires for a projective manifold M (i.e., a compact complex manifold with an embedding into $\mathbb{C}P^{n-1}$) that the action of G extends to a linear action on $\mathbb{C}P^{n-1}$. Thus, moment maps for such linear actions are given by [3] composed with π and with the embedding of M into $\mathbb{C}P^{n-1}$ (see also Cotangent Bundle Reduction, Poisson Reduction, Symmetry and Symplectic Reduction).

Reduction in Stages

Suppose a compact Lie group G acts in a Hamiltonian fashion on a symplectic manifold M , and H is a normal subgroup of G . (For example, this hypothesis is satisfied if both H and G are tori.) Suppose also that 0 is a regular value for μ_H and μ_G . Then the symplectic quotient $\mu_H^{-1}(0)/H$ is acted on naturally by the quotient group G/H , and this action is Hamiltonian; furthermore, the symplectic quotient of $\mu_H^{-1}(0)/H$ by G/H is naturally isomorphic to $\mu_G^{-1}(0)/G$. (This result is known as “reduction in stages.”)

Let M be a symplectic manifold equipped with the Hamiltonian action of a torus T . Let $H \subset T$ be a Lie subgroup of T (so H is a torus whose dimension is smaller than the dimension of T). Let $\mu_T: M \rightarrow \text{Lie}(T)^*$ and $\mu_H: M \rightarrow \text{Lie}(H)^*$ be the moment maps: recall that $\mu_H = \pi_H \circ \mu_T$, where $\pi_H: \text{Lie}(T)^* \rightarrow \text{Lie}(H)^*$ is the standard projection.

For any $\eta \in \text{Lie}(H)^*$ we may form the reduced space $M_\eta = \phi_H^{-1}(\eta)/H$. This is equipped with a Hamiltonian action of T/H .

Example 9 Let $U(n)$ act on \mathbb{C}^n in the standard way. This action descends to an action on $\mathbb{C}P^{n-1}$, which is the symplectic quotient of \mathbb{C}^n under the action of the diagonal $U(1)$ subgroup of $U(n)$. Hence, the moment map $\hat{\mu}$ for the action of $U(n)$ on $\mathbb{C}P^{n-1}$ is given by the formula

$$\hat{\mu}([z_1, \dots, z_n])_{jk} = \frac{i}{2} \frac{z_j \bar{z}_k}{\sum_{\ell=1}^n |z_\ell|^2} \quad [3]$$

which comes from the moment map [2] for the action of $U(n)$ on \mathbb{C}^n .

The Normal Form Theorem

There is a neighborhood of $\mu^{-1}(0)$ on which the symplectic form is given in a standard way related to the symplectic form ω_0 on M_{red} (see, e.g., Guillemin and Sternberg (1990, sections 39–41)).

Proposition 3 (Normal form theorem). *Assume 0 is a regular value of μ (so that $\mu^{-1}(0)$ is a smooth manifold and G acts on $\mu^{-1}(0)$ with finite stabilizers). Then there is a neighborhood $U \cong \mu^{-1}(0) \times \{z \in \mathfrak{g}^*, |z| \leq h\}$ of $\mu^{-1}(0)$ on which the symplectic form is given as follows. Let $P \stackrel{\text{def}}{=} \mu^{-1}(0) \overset{q}{\rightarrow} M_{\text{red}}$ be the orbifold principal G -bundle given by the projection map $q: \mu^{-1}(0) \rightarrow \mu^{-1}(0)/G$, and let $\theta \in \Omega^1(P) \otimes \mathfrak{g}$ be a connection for it. Let ω_0 denote the induced symplectic form on M_{red} , in other words $q^* \omega_0 = i_0^* \omega$. Then if we define a 1-form τ on $U \subset P \times \mathfrak{g}^*$ by $\tau_{p,z} = z(\theta)$ (for $p \in P$ and $z \in \mathfrak{g}^*$), the symplectic form on U is given by*

$$\omega = q^* \omega_0 + d\tau \quad [4]$$

Further, the moment map on U is given by $\mu(p, z) = z$.

Corollary 3 *Let t be a regular value for the moment map for the Hamiltonian action of a torus T on a symplectic manifold M . Then in a neighborhood of t , all symplectic quotients M_t are diffeomorphic to M_{t_0} by a diffeomorphism under which $\omega_t = \omega_{t_0} + (t - t_0, d\theta)$ where $\theta \in \Omega^1(\mu^{-1}(t_0)) \otimes \mathfrak{t}$ is a connection for the action of T on $\mu^{-1}(t_0)$.*

Corollary 4 *Suppose G acts in a Hamiltonian fashion on a symplectic manifold M , and suppose 0 is a regular value for the moment map μ . Then the reduced space $M_\lambda = \mu^{-1}(\mathcal{O}_\lambda)/G$ at the orbit \mathcal{O}_λ fibers over $M_0 = \mu^{-1}(0)/G$ with fiber the orbit \mathcal{O}_λ ; furthermore, if $\pi: M_\lambda \rightarrow M_0$ is the projection map, then the symplectic form ω_λ on $\mu^{-1}(\mathcal{O}_\lambda)/G$ is given as $\omega_\lambda = \pi^* \omega_0 + \Omega_\lambda$, where ω_0 is the symplectic form on M_0 and Ω_λ restricts to the standard Kirillov–Kostant symplectic form on the fiber.*

Convexity Theorems

Theorem 1 (Atiyah (1982); Guillemin–Sternberg (1982 and 1984)). *Suppose M is a connected compact symplectic manifold equipped with a Hamiltonian action of a torus T . Then the image $\mu(M)$ is a convex polytope, the convex hull of $\{\mu(F)\}$, where F are the components of the fixed-point set of T in M .*

Example 10 Consider the orbits \mathcal{O}_t of $SU(2)$ in $\mathfrak{su}(2) \cong \mathbb{R}^3$ through $t \in \mathbb{R}^+$. The image of the moment map for the action of the maximal torus $T \cong U(1)$ is the interval $[-t, t]$.

Example 11 When \mathcal{O}_t is the coadjoint orbit (through $t \in \mathfrak{t}^*$) for a compact Lie group G with maximal torus T , the image $\mu_T(\mathcal{O}_t)$ of the moment map μ_T for the action of the maximal torus T is the convex hull $\text{Conv}\{wt : w \in W\}$, where W is the Weyl group.

The convexity theorem above can be generalized to actions of nonabelian groups. If M is a connected compact symplectic manifold equipped with a Hamiltonian action of a compact Lie group G with maximal torus T and positive Weyl chamber \mathfrak{t}_+ , then the intersection of the image $\mu(M)$ of the moment map with the positive Weyl chamber \mathfrak{t}_+ (in other words, a fundamental domain for the action of the Weyl group on \mathfrak{t}) is a convex polytope. This result is due to Kirwan (1984b) and for Kähler manifolds to Guillemin and Sternberg (1982 and 1984).

The proofs of Atiyah and Guillemin–Sternberg are based on Morse theory applied to the moment map. A key ingredient in the proofs is to establish that the fibers of the moment map are connected.

The Moment Polytope

Given a compact symplectic manifold M equipped with the Hamiltonian action of a torus T , we see that there is an associated polytope P , the “moment polytope.” The fibers of the moment map μ are preserved by the action of T , so the value of μ parametrizes a family $\{M_t\}$ of symplectic quotients. By Theorem 1 the moment polytope is the convex hull of the images of the fixed-point set under the moment map.

By Proposition 1, we see that the moment polytope is decomposed according to the stabilizers of points in the preimage, and the critical values of the moment map are the images $\mu_T(W_j)$ of the fixed-point sets W_j of one-parameter subgroups S_j of T . These critical values form hyperplanes (“walls”) which subdivide the moment polytope: the complement of the walls is a collection of open regions consisting of regular values of the moment map.

Example 12 The group $SU(3)$ has maximal torus $T \cong U(1)^2$. We identify \mathfrak{g}^* with \mathfrak{g} via the bi-invariant inner product (i.e., the Killing form) on \mathfrak{g} , and thus identify \mathfrak{t}^* with \mathfrak{t} . For $\lambda \in \mathfrak{t}$, the Weyl group images of λ are the six vertices of a hexagon: the “walls” in the moment polytope for the action of T on the coadjoint orbit \mathcal{O}_λ arising from the action of G on \mathfrak{g}^* through $\lambda \in \mathfrak{t}^*$ are the edges of the hexagon (exterior walls) and the three lines connecting opposite vertices (interior walls).

Toric Manifolds

Definition 1 A toric manifold is a compact symplectic manifold M of dimension $2n$ equipped with the effective Hamiltonian action of a torus T of dimension n .

Example 13 Complex projective space CP^n with the obvious Hamiltonian action of $U(1)^n \subset U(1)^{n+1}$ is a toric manifold.

Example 14 A special case of Example 13 is the 2-sphere $S^2 \cong CP^1$ (with the action of $U(1)$ given by rotation around one axis). The 2-sphere is a toric manifold.

Elementary Properties of Toric Manifolds

If M is a toric manifold, the fiber of the moment map for the action of T is an orbit of the action. Hence, the symplectic quotient M_t at any value $t \in \mathfrak{t}^*$ is a point (if it is nonempty).

The regular values of μ are the interior points of the moment polytope P . All points in the preimage $\mu^{-1}(\partial P)$ are fixed points of some one-parameter subgroup of T . Points in the interior of a face P_j of dimension j are fixed by a subtorus of T of dimension $n - j$. Hence, each fiber of μ over a point in P_j is a quotient torus of dimension j . In particular, the vertices of the polytope are the images of the components of the fixed-point set of the whole torus T , and the inverse image of a vertex is contained in the fixed-point set of T .

The push-forward function $\mu_*(\omega^n/n!)$ under the moment map is just the characteristic function of the moment polytope.

Delzant's Theorem

In fact, toric manifolds are characterized by their moment polytopes. A theorem of Delzant (1988) says that any polytope P satisfying appropriate hypotheses (a simple polytope) is the moment polytope for some toric manifold; furthermore, if two toric manifolds acted on effectively by a torus T have the same moment polytope, then they are T -equivariantly symplectomorphic. The first statement is proved by constructing a toric manifold which has the polytope P as its moment polytope; if P has d faces of codimension 1, one constructs the toric manifold M as a symplectic quotient of a vector space $V \cong \mathbb{C}^d$ by the linear action of a torus $T' \cong U(1)^{d-n}$. The torus $T \cong U(1)^n$ acting on M is then obtained by reduction in stages, as the quotient of $U(1)^d$ by T' .

The construction of a toric manifold whose moment polytope is a given simple polytope is

given in Guillemin (1994, chapter 1). The second statement (namely that toric manifolds are classified by their moment polytopes) is proved in Delzant (1988).

Example 15 The moment polytope for the action of $U(1)^n$ on CP^n is the n -simplex. This action descends from the action of $U(1)^{n+1}$ on C^{n+1} , using reduction in stages: recall from Example 5 that we constructed CP^n as the symplectic quotient of C^{n+1} by the standard action of $U(1)$.

Cohomology Rings of Symplectic Quotients

For material on the equivariant cohomology of symplectic manifolds equipped with Hamiltonian group actions and the relation to the fixed-point set, we refer to *Equivariant Cohomology and the Cartan Model*. As in that reference we shall describe the equivariant cohomology of a Hamiltonian G -manifold using the Cartan model.

Two fundamental results of Kirwan give complementary descriptions of the equivariant cohomology of a symplectic manifold.

Kirwan Injectivity

Kirwan's first theorem is the injectivity theorem:

Theorem 2 (Injectivity theorem). *If T is a compact torus and M is a Hamiltonian T -space, then the direct sum of restriction maps to all components of the fixed-point set*

$$\oplus_F : H_T^*(M) \rightarrow H^*(F) \otimes S(\mathfrak{t}^*)$$

is injective.

The proof appears in Kirwan (1984a); this material is treated in *Equivariant Cohomology and the Cartan Model* (theorem 6.6).

Kirwan Surjectivity

Let G be a complex torus, and let 0 be a regular value of the moment map μ . Suppose M is a compact symplectic manifold equipped with a Hamiltonian action of a compact Lie group G . There is a natural map $\kappa : H_G^*(M) \rightarrow H^*(M_{\text{red}})$ defined by

$$\kappa : H_G^*(M) \mapsto H_G^*(\mu^{-1}(0)) \cong H^*(M_{\text{red}})$$

(where the first map is the restriction map and the second is the identification of $H_G^*(Z)$ with $H^*(Z/G)$ when G acts locally freely on Z and the cohomology is taken with rational coefficients). The map κ is

obviously a ring homomorphism. Kirwan's second theorem treats the image of κ .

Theorem 3 (Surjectivity theorem). *Under the above hypotheses, the map κ is surjective.*

The proof of this theorem (Kirwan (1984a, 5.4 and 8.10); see also Kirwan (1992, section 6)) uses the Morse theory of the "Yang–Mills function" $|\mu|^2 : M \rightarrow \mathbb{R}$ to define an equivariant stratification of M by strata S_β which flow under the gradient flow of $|\mu|^2$ to a critical set C_β of $|\mu|^2$. One shows that the function $|\mu|^2$ is equivariantly perfect (i.e., that the Thom–Gysin (long) exact sequence in equivariant cohomology decomposes into short exact sequences, so that one may build up the cohomology as

$$H_G^*(M) \cong H_G^*(\mu^{-1}(0)) \oplus \bigoplus_{\beta \neq 0} H_G^*(S_\beta)$$

Here, the stratification by S_β has a partial order $>$; thus, one may define an open dense set $U_\beta = M - \bigcup_{\gamma > \beta} S_\gamma$ which includes the open dense stratum S_β of points that flow into $\mu^{-1}(0)$ (note S_β retracts onto $\mu^{-1}(b)$). The equivariant Thom–Gysin sequence is

$$\cdots \rightarrow H_G^{n-2d(\beta)}(S_\beta) \xrightarrow{i_{\beta*}} H_G^n(U_\beta) \rightarrow H_G^n(U_\beta - S_\beta) \rightarrow \cdots$$

To show that the Thom–Gysin sequence splits into short exact sequences, it suffices to know that the maps $(i_\beta)_*$ are injective. Since $i_\beta^*(i_\beta)_*$ is multiplication by the equivariant Euler class e_β of the normal bundle to S_β , injectivity follows because this equivariant Euler class is not a zero divisor (see Kirwan (1984a, 5.4) for the proof).

Because κ is a surjective ring homomorphism, it follows that

$$H_G^*(M_{\text{red}}) \cong H_T^*(M)/\text{Ker}(\kappa)$$

The above theorem is also valid when G is the complexification of a compact semisimple Lie group. In this case, one must reduce at 0 (because of the condition that the moment map is equivariant, since $b=0$ is the only value which is invariant under the coadjoint action). The case of reducing at coadjoint orbits can be treated using the proof for the case of reducing at 0 via the shifting trick (Example 8).

Several recent articles (Jeffrey and Kirwan (1995, 1997), Tolman and Weitsman 2003) compute $\text{Ker}(\kappa)$. Some articles compute $\text{Ker}(\kappa)$ in specific examples, notably the action of S^1 on products of two-dimensional spheres of general radii.

The Residue Formula

One approach to identifying $\text{Ker}(\kappa)$ is the "residue formula," Jeffrey and Kirwan (1995), theorem 8.1:

Theorem 4 (Jeffrey and Kirwan (1995), corrected as in Jeffrey and Kirwan (1997)).

Let $\eta \in H_G^*(M)$ induce $\eta_0 \in H^*(M_{\text{red}})$. Then we have

$$\int_{M_{\text{red}}} \kappa(\eta) e^{i\omega_{\text{red}}} = n_0 C^G \text{Res} \left(\mathcal{D}^2(X) \sum_{F \in \mathcal{F}} h_F^\eta(X) [dX] \right) \quad [5]$$

where n_0 is the order of the stabilizer in G of a generic element of $\mu^{-1}(0)$, and the constant C^G is defined by

$$C^G = \frac{(-1)^{s+n_+}}{|W| \text{vol}(T)} \quad [6]$$

We have introduced $s = \dim G$ and $l = \dim T$; here $n_+ = (s - l)/2$ is the number of positive roots. Also, \mathcal{F} denotes the set of components of the fixed-point set of T , and if F is one of these components, then the meromorphic function h_F^η on $\mathfrak{t} \otimes \mathbb{C}$ is defined by

$$h_F^\eta(X) = e^{i\mu(F)(X)} \int_F \frac{i_F^* \eta(X) e^{i\omega}}{e_F(X)} \quad [7]$$

and the polynomial $\mathcal{D}: \mathfrak{t} \rightarrow \mathbb{R}$ is defined by $\mathcal{D}(X) = \prod_{\gamma > 0} \gamma(X)$, where γ runs over the positive roots of G .

The residue map Res is defined on (a subspace of) the meromorphic differential forms on $\mathfrak{t} \otimes \mathbb{C}$: its definition depends on some choices, but the sum of the residues over all $F \in \mathcal{F}$ is independent of these choices. When $T = U(1)$, we define the residue on meromorphic functions of the form $e^{i\lambda X}/X^N$ when $\lambda \neq 0$ (for $N \in \mathbb{Z}$) by

$$\begin{aligned} \text{Res} \left(\frac{e^{i\lambda X}}{X^N} \right) &= \text{Res}_{X=0} \frac{e^{i\lambda X}}{X^N}, \quad \text{if } \lambda > 0 \\ &= 0, \quad \text{if } \lambda < 0 \end{aligned}$$

More generally, the residue is specified by certain axioms (see Jeffrey and Kirwan (1995, proposition 8.11)), and may be defined as a sum of iterated multivariable residues $\text{Res}_{X_1=\lambda_1} \dots \text{Res}_{X_l=\lambda_l}$ for a suitably chosen basis of \mathfrak{t} yielding coordinates X_1, \dots, X_l (see Jeffrey and Kirwan (1997)).

The Tolman–Weitsman Theorem

The Tolman and Weitsman (2002) theorem is as follows:

Theorem 5 We have

$$\text{Ker}(\kappa) = \sum_S (K_-^S \oplus K_+^S) \quad [8]$$

Here, S is a generic circle subgroup of T and K_-^S (resp. K_+^S) denote the set of all equivariant cohomology classes η whose restriction to \mathcal{F}_-^S (resp. \mathcal{F}_+^S) is zero. Here,

$$\mathcal{F}_\pm = \{F \in \mathcal{F} : \pm \mu_S(F) > 0\}$$

where μ_S is the component of the moment map in the direction of the Lie algebra of S .

For more information, see Intersection Theory, Moduli Spaces: An Introduction, and Equivariant Cohomology and the Cartan Model.

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See also: Cotangent Bundle Reduction; Equivariant Cohomology and the Cartan Model; Hamiltonian Fluid Dynamics; Intersection Theory; Moduli Spaces: An Introduction; Poisson Reduction; Stationary Phase Approximation; Symmetry and Symplectic Reduction.

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Hamiltonian Reduction of Einstein's Equations

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Further information and details regarding the authors' work discussed in this article can be found in Fischer and Moncrief (2000, 2002a, b) and in the references therein.

Introduction

In general relativity there are several levels within the framework of symplectic reduction of Einstein's equations at which one could attempt to define a Hamiltonian for the gravitational dynamics of a spatially closed universe. At the most basic unreduced level, this Hamiltonian is simply a linear function of the Einstein constraints and thus vanishes for any solution of the field equations. At the other extreme, at the deepest fully reduced level, one affects a transformation to a complete set of new canonical variables, the so-called "observables," which Poisson-commute with all of the constraints. At this level, the relevant Hamiltonian vanishes identically since each of the new canonical variables is a constant of the motion.

There is, however, an intermediate level wherein, after making a suitable choice of coordinate gauge and imposing the constraint equations, one can define a nonvanishing Hamiltonian that generates the gauge-fixed and constrained evolution equations and whose global infimum as a function on the relevant reduced phase space has direct topological significance. For the large class of manifolds on which this Hamiltonian can be defined, it has the attractive feature of globally monotonically decaying in the direction of cosmological expansion and thus evolves in such a way so as to seek and, in certain cases at least, to asymptotically attain its infimum value in the limit of this expansion. This Hamiltonian provides in these cases a weak Lyapunov function for the dynamics that can be used to partially control its global behavior. Since understanding the global behavior of solutions to Einstein's equations and its dependence upon the spatial topology is one of the central open problems in classical general relativity, the mathematical properties of this quantity are worthy of study.

Topological Background

Einstein's field equations are nonvacuous and compatible with the introduction of material sources in $(n+1)$ dimensions for all $n \geq 2$, the case of most physical interest being of course $n=3$. For the field equations to be deterministic in a classical sense, that is, for the Cauchy problem to be well-posed, it is essential that they be formulated on a manifold that is globally hyperbolic and, in particular, has a product topology $M \times \mathbb{R}$ (roughly, space \times time = spacetime) where M is a smooth (C^∞) connected manifold of dimension n and \mathbb{R} is the real line. For the case of spatially closed universes of interest here, M should be closed, that is, compact and without boundary. To simplify the analysis further, we also assume that M is oriented, that is, orientable and an orientation has been chosen. Thus, unless stated otherwise, throughout this article M will denote a smooth closed connected oriented n -manifold, $n \geq 2$, and all maps will be smooth.

Let " \approx " denote the diffeomorphic equivalence relation between smooth manifolds. Let S^n denote the unit n -sphere in Euclidean $(n+1)$ space \mathbb{R}^{n+1} , $n \geq 1$. An n -manifold M is trivial if $M \approx S^n$ and nontrivial if $M \not\approx S^n$.

The connected sum $M \# N$ of two closed connected oriented n -manifolds M and N is constructed by removing the interior of an embedded closed n -ball in M and N , respectively, and then identifying the resulting S^{n-1} -boundary components by an orientation-reversing diffeomorphism of the $(n-1)$ spheres. The resulting manifold is smooth, connected, closed, and orientable, and is naturally oriented by the orientations on M and N . Up to orientation-preserving diffeomorphism, this construction is independent of the choice of the embeddings of the n -balls and of the choice of the orientation-reversing diffeomorphism used to join the manifolds together.

Let M be a nontrivial closed connected oriented n -manifold. Then M is prime if $M \approx M_1 \# M_2$ implies that either $M_1 \approx S^n$ or $M_2 \approx S^n$ (but not both since we are assuming that M is nontrivial). M is a composite if M can be written as a nontrivial connected sum, that is, if $M \approx M_1 \# M_2$ where both $M_1 \not\approx S^n$ and $M_2 \not\approx S^n$.

Note that with this definition, S^n itself is not prime. This is analogous to the fact that for the positive integers, the unit 1 is not prime.

Now let M be a connected n -manifold without boundary (not necessarily compact or orientable) and let π be a group. Then M is a $K(\pi, 1)$ -manifold if M is an Eilenberg–MacLane space, that is, if its first homotopy group (or fundamental group) $\pi_1(M) = \pi$ and if all of its higher homotopy groups are trivial, that is, $\pi_i(M) = 0$ for $i > 1$ (equivalently, the universal covering space \tilde{M} of M is contractible). Since the higher homotopy groups $\pi_i(M)$, $i > 1$, can be interpreted as the homotopy classes of continuous maps $S^i \rightarrow M$, each such map must be homotopic to a constant map. Thus a $K(\pi, 1)$ -manifold is said to be aspherical. Moreover, at the level of homotopy, all of the information about the topology of M is contained in $\pi_1(M) = \pi$. Thus, in particular, if f is a map between connected aspherical manifolds that induces an isomorphism on their fundamental groups, then f is a homotopy equivalence. Consequently, any two connected aspherical manifolds are homotopy equivalent if and only if their fundamental groups are isomorphic.

It is useful to define a connected n -manifold M to be hyperbolizable if there exists a complete Riemannian metric g on M with constant negative sectional curvature, $K(g) = \text{constant} < 0$. We introduce this terminology to emphasize the underlying topology of manifolds that can support hyperbolic metrics rather than the geometry of such metrics. Similarly, M is of flat type if M admits a complete flat Riemannian metric g , $K(g) = 0$, and M is of spherical type if M admits a complete Riemannian metric g on M with constant positive sectional curvature, $K(g) = \text{constant} > 0$. In this latter case, by the Bonnet–Myers theorem, M is necessarily compact and if n is odd, then by Synge's theorem, M is necessarily orientable. In fact, all such manifolds have been classified. As an important example, we note that a connected 3-manifold M is of spherical type if and only if it is diffeomorphic to a spherical space form S^3/Γ , where Γ is a finite subgroup of $\text{SO}(4)$ acting freely and orthogonally, that is, isometrically, on S^3 .

Within the class of $K(\pi, 1)$ -manifolds are all flat-type and hyperbolizable n -manifolds, since any such manifold is isometrically covered by \mathbb{R}^n in the flat case and homothetically covered by H^n in the hyperbolic case, where H^n is the standard single-sheeted spacelike

hyperboloid with constant sectional curvature $K = -1$ embedded in $(n+1)$ -Minkowski space \mathbb{R}_1^{n+1} .

We now return to our standard assumptions on M , so that M is connected, closed, and oriented. For $n=2$, these assumptions restrict the possibilities to S^2 , T^2 , and the orientable higher genus surfaces $\Sigma_p^2 = T^2 \# T^2 \# \cdots \# T^2$ (p factors) consisting of the connected sum of p copies of T^2 , $p \geq 2$. However, from the point of view of $(2+1)$ gravity, unless one includes material sources or a cosmological constant, the spherical case is vacuous in that there are no vacuum solutions of the field equations on $S^2 \times \mathbb{R}$. The torus case is nonvacuous but the solutions, the so-called flat Kazner spacetimes, can all be found by elementary means. Thus only the case of genus $p \geq 2$ surfaces presents problems of interest.

For $n=3$, although not essential for the program of reduction, it is convenient to assume the elliptization conjecture of 3-manifold topology. This conjecture asserts that a closed connected 3-manifold M with finite fundamental group $\pi_1(M)$ must be diffeomorphic to a spherical space form S^3/Γ , where, in such a quotient, Γ will always be a finite subgroup of $\text{SO}(4)$ acting freely and orthogonally on S^3 and thus Γ is isomorphic to $\pi_1(M)$.

The simply connected case is the Poincaré conjecture. The full elliptization conjecture is equivalent to the Poincaré conjecture and a conjecture asserting that the only free actions of finite groups on S^3 are equivalent to the standard orthogonal ones. The elliptization conjecture is part of Thurston's geometrization program (Thurston 1997). For background information regarding 3-manifold topology, see Hempel (1976) and Jaco (1980).

Under the assumption of the elliptization conjecture, the Kneser–Milnor prime decomposition theorem asserts that if M is nontrivial, then up to order, M is uniquely diffeomorphic to a finite connected sum of the following form:

$$M \approx \underbrace{\left(S^3/\Gamma_1 \# \cdots \# S^3/\Gamma_k \right)}_{k \text{ spherical factors}} \# \underbrace{\left((S^1 \times S^2) \# \cdots \# (S^1 \times S^2) \right)}_{l \text{ wormholes (or handles)}} \# \underbrace{\left(K(\pi_1, 1) \# \cdots \# K(\pi_m, 1) \right)}_{m \text{ aspherical factors}} \quad [1]$$

where k , l , and m are integers ≥ 0 , $k+l+m \geq 1$, and if either k , l , or m is 0, terms of that type do not appear. Moreover, if $k \geq 1$, then each Γ_i , $1 \leq i \leq k$, is a finite nontrivial ($\Gamma_i \neq \{I\}$) subgroup of $\text{SO}(4)$

acting freely and orthogonally on S^3 , and if $m \geq 1$, then each aspherical factor is a $K(\pi_j, 1)$ -manifold, $1 \leq j \leq m$, and thus is universally covered by a contractible manifold.

We remark that although in general a contractible 3-manifold need not be R^3 , conjecturally the universal covering manifold of a $K(\pi, 1)$ 3-manifold is diffeomorphic to R^3 .

In 3-manifold topology, a concept closely related to that of a prime manifold is that of an irreducible manifold. A closed 3-manifold M is irreducible if every embedded 2-sphere in M is the boundary of an embedded closed 3-ball.

An embedded 2-sphere that does not bound such a 3-ball is essential. Thus in the prime decomposition [1] above, M is decomposed along essential 2-spheres. For this reason, the prime decomposition is sometimes referred to as the sphere decomposition.

With the exception of S^3 which is irreducible but not prime (by definition of prime) and $S^1 \times S^2$ which is prime but not irreducible, a closed oriented 3-manifold is prime if and only if it is irreducible. We also remark that the Poincaré conjecture, when taken in the form that there do not exist any fake 3-cells, is equivalent to every $K(\pi, 1)$ 3-manifold being irreducible. Thus in this article, since we are assuming the elliptization conjecture and hence the Poincaré conjecture, every $K(\pi, 1)$ 3-manifold will automatically be irreducible.

Examples of the kinds of $K(\pi, 1)$ -factors that can occur in the decomposition [1] are as follows (we will explain the Seifert and graph designations below):

1. **Non-Seifert manifolds.** Closed oriented hyperbolizable manifolds diffeomorphic to H^3/Γ , where Γ is a discrete torsion-free (i.e., no nontrivial element has finite order) co-compact subgroup of the Lie group $\text{Isom}^+(H^3)$ of orientation-preserving isometries of H^3 which is Lie-group isomorphic to the proper orthochronous Lorentz group $\text{SO}^+(1, 3)$.
2. **Seifert manifolds.** T^3 and five other 3-manifolds of flat type which are finitely covered by T^3 . Noting that $\Sigma_1^2 = T^2$, we remark that the product manifold $S^1 \times \Sigma_1^2 = S^1 \times T^2 = T^3$ is included in this class.
3. **Seifert manifolds.** Product manifolds $S^1 \times \Sigma_p^2$, $p \geq 2$.
4. **Seifert manifolds.** Nontrivial circle bundles over Σ_p^2 , $p \geq 1$.
5. **Graph manifolds.** Any 3-manifold which fibers nontrivially over a circle with fiber Σ_p^2 , $p \geq 1$. Any such manifold is obtained by identifying the boundary components of $[0, 1] \times \Sigma_p^2$ with an orientation-reversing diffeomorphism of Σ_p^2 .

Since the handle $S^1 \times S^2$ and spherical manifolds S^3/Γ are well understood, under the assumption of the elliptization conjecture the task of 3-manifold

topology now reduces to understanding the topology of the (automatically irreducible) $K(\pi, 1)$ -factors that can occur in the prime decomposition [1]. Since essential 2-spheres have already been used to decompose M into its prime components, the idea now is to use the next simplest 2-manifold, the 2-torus, to probe the irreducible $K(\pi, 1)$ -factors.

Let $i: T^2 \rightarrow M$ be an embedding of T^2 into a closed oriented 3-manifold M . Then the embedded torus $i(T^2)$, identified with T^2 , is incompressible if the induced mapping of fundamental groups $i_*: \pi_1(T^2) \rightarrow \pi_1(M)$ is injective. Thus noncontractible loops in T^2 remain noncontractible when T^2 is embedded in M , or, in other words, the ambient manifold M does not fill in any homotopy hole that exists in T^2 when standing alone.

A closed oriented 3-manifold M is a Seifert-fibered space, or a Seifert manifold, if M admits a foliation by circles. For example, if S^1 acts freely on M , then M is the total space of an S^1 -bundle over a surface M/S^1 and M is a Seifert-fibered space (see examples 2, 3, and 4 above). More generally, if S^1 acts without fixed points (locally free), then M is a Seifert-fibered space, and in either case the fibers of M are the orbits of the S^1 -action.

All spherical 3-manifolds are Seifert fibered with base S^2 . Also, the product manifold $S^1 \times S^2$ is Seifert fibered, as are all manifolds finitely covered by T^3 , and thus all 3-manifolds of flat type are Seifert fibered. The only nontrivial connected sum that is a Seifert-fibered space is $P^3 \# P^3$. No hyperbolizable manifold is Seifert fibered. Thus the remaining Seifert manifolds are among the nonhyperbolizable nonflat type $K(\pi, 1)$ -manifolds (i.e., those for which M does not admit either a hyperbolic or a flat Riemannian metric).

A generalization of Seifert-fibered spaces are the graph manifolds. A closed oriented 3-manifold M is a graph manifold if there exists a finite collection $\{T_i^2\}$ of disjoint embedded incompressible tori $T_i^2 \subset M$ such that each component M_i of $M \setminus \bigcup T_i^2$ is a Seifert-fibered space. Thus a graph manifold is a union of Seifert-fibered spaces glued together by toral automorphisms along toral boundary components. The collection of tori may be empty so that, in particular, a Seifert-fibered manifold is a graph manifold.

We remark that the manifolds described by example 5 above are graph manifolds. We also remark that graph manifolds are closed under connected sums so that a graph manifold may be a composite. This contrasts with the situation for Seifert spaces which, with the exception of $P^3 \# P^3$, are not composites.

Conjecturally, the most general $K(\pi, 1)$ -manifold, not included in the list above, consists of "gluing together" across disjoint embedded incompressible

tori a finite collection of finite-volume-type hyperbolizable manifolds, that is, noncompact manifolds that admit a finite-volume complete hyperbolic metric, together with a possibly empty finite collection of irreducible graph manifolds with toral boundaries. Thus, overall, in this picture, to decompose an arbitrary closed oriented 3-manifold M into its elementary constituents, one first cuts along essential 2-spheres to break M down into its prime factors, that is, the nontrivial spherical S^3/Γ -factors, the wormhole $(S^1 \times S^2)$ -factors, and the aspherical $K(\pi, 1)$ -factors, as given by [1]. Then one cuts each nonelementary $K(\pi, 1)$ -factor along incompressible tori to separate these factors into their final finite-volume-type hyperbolizable and irreducible graph manifold components. The graph manifold components can then be further broken down along incompressible tori into Seifert-fibered pieces, finally yielding the toral decomposition of Jaco, Shalen, and Johannson (see Anderson (1997), Jaco (1980), and the end of the section "The Reduced Hamiltonian" for further details).

The Thurston (1997) geometrization program, which implies that every closed oriented 3-manifold has the structure described by the above prime (or spherical) and toroidal decomposition, has been the subject of recent work by G Perelman (see Anderson (2003) and the references therein) who has argued that it can be proved by an enhancement of the Ricci flow program of R Hamilton (see the collected papers edited by Cao *et al.* (2003)). Without entering into the technical issues surrounding the completeness of Perelman's proof, one can simply limit one's attention to 3-manifolds of the above type. If geometrization is correct, then no 3-manifolds of interest have been excluded.

Returning to the general case of n -manifolds, in the program of Hamiltonian reduction of Einstein's equations, an important consideration is under what topological conditions on M can the conformal classes of M be uniquely represented by a given metric in each class. To analyze that question, we introduce the concept of the Yamabe type of a manifold.

Let M be a connected closed oriented n -manifold, $n \geq 3$. There is no topological obstruction to the existence of Riemannian metrics with constant negative scalar curvature, so all such manifolds admit a Riemannian metric g such that $R(g) = -1$. However, there are topological obstructions for zero scalar curvature and positive constant scalar curvature metrics on M . To help categorize these topological obstructions, we introduce the following terminology:

1. M is of *positive Yamabe type* if M admits a Riemannian metric g_1 with scalar curvature $R(g_1) = 1$;

2. M is of *zero Yamabe type* if M admits a Riemannian metric g_0 with $R(g_0) = 0$, but no Riemannian metric g with $R(g) = 1$; and
3. M is of *negative Yamabe type* if M admits no Riemannian metric g with $R(g) = 0$.

The definition of Yamabe type partitions the class of connected closed oriented n -manifolds, $n \geq 3$, into three classes that are mutually exclusive and exhaustive. The following rather complete topological information regarding 3-manifolds of negative Yamabe type is known.

Let M be a connected closed oriented 3-manifold. Assume that the Poincaré conjecture is true. Then M is of negative Yamabe type if and only if M satisfies one of the following three mutually exclusive conditions:

1. M is hyperbolizable (and thus is a $K(\pi, 1)$ -manifold; see example 1 of $K(\pi, 1)$ -manifolds);
2. M is a nonhyperbolizable nonflat type $K(\pi, 1)$ -manifold (see examples 3, 4, and 5 of $K(\pi, 1)$ -manifolds);
3. M has a nontrivial connected sum decomposition (i.e., M is a composite) in which at least one factor is a $K(\pi, 1)$ -manifold; that is, $M \approx M' \# K(\pi, 1)$, where $M' \not\approx S^3$. In this case the $K(\pi, 1)$ -factor may be either of flat type or hyperbolizable.

We remark that (1) is the vast class of closed oriented hyperbolizable 3-manifolds. We also remark that the six closed orientable 3-manifolds of flat type, although $K(\pi, 1)$ -manifolds, are excluded from (2) as they are not of negative Yamabe type (they are of zero Yamabe type). Lastly we remark that if M is of negative Yamabe type and Seifert fibered, then M must be of type (2) (see remarks on Seifert-fibered spaces above).

In any dimension $n \geq 3$, a manifold M of negative Yamabe type has the property that it admits no Riemannian metric g having scalar curvature $R(g) \geq 0$ everywhere on M , or, in other words, every Riemannian metric on M has scalar curvature which is negative somewhere. For such a manifold M , Yamabe's theorem asserts that each Riemannian metric g on M is uniquely globally conformal to a metric γ with scalar curvature $R(\gamma) = -1$ (see also [21]). Thus one can represent the conformal classes of Riemannian metrics on M in a suitable function space setting by an infinite-dimensional submanifold

$$\mathcal{M}_{-1} = \mathcal{M}_{-1}(M) = \{\gamma \in \mathcal{M} \mid R(\gamma) = -1\} \quad [2]$$

of the space $\mathcal{M} = \mathcal{M}(M) = \text{Riem}(M)$ of Riemannian metrics on M (see Fischer and Marsden (1975) for details). For this reason, we refer to metrics γ in \mathcal{M}_{-1} as conformal metrics.

The quotient of \mathcal{M}_{-1} by the natural action of $\mathcal{D}_0 = \mathcal{D}_0(M) = \text{Diff}_0(M)$, the connected component of the identity of the diffeomorphism group $\mathcal{D} = \mathcal{D}(M) = \text{Diff}(M)$ of M , defines an orbit space (not necessarily a manifold) $\mathcal{T} = \mathcal{T}(M)$,

$$\mathcal{T} = \frac{\mathcal{M}_{-1}}{\mathcal{D}_0} \quad [3]$$

which, when M is of negative Yamabe type, we define as the Teichmüller space of conformal structures on M .

In two dimensions in the case of a higher genus manifold Σ_p^2 , $p \geq 2$, this construction leads precisely to the conventional Teichmüller space, as discussed by Fischer and Tromba (1984). In this case the resulting Teichmüller space

$$\mathcal{T}_p = \mathcal{T}(\Sigma_p^2) = \frac{\mathcal{M}_{-1}(\Sigma_p^2)}{\mathcal{D}_0(\Sigma_p^2)} \approx \mathbb{R}^{6p-6} \quad [4]$$

is then a manifold diffeomorphic to \mathbb{R}^{6p-6} , which then plays the role of the natural reduced configuration space for the Einstein equations in $(2+1)$ dimensions. Moreover, these constructions can be carried out globally using known global cross sections for the $\mathcal{D}_0(\Sigma_p^2)$ action on $\mathcal{M}_{-1}(\Sigma_p^2)$. These global cross sections can then be used to provide an explicit model for the Teichmüller space \mathcal{T}_p as a finite-dimensional subspace of $\mathcal{M}_{-1}(\Sigma_p^2)$.

For $n=3$, $\mathcal{T} = \mathcal{T}(M)$ plays the analogous role for the reduced field equations in $(3+1)$ dimensions. Moreover, for many 3-manifolds it is possible to show that \mathcal{T} is itself an infinite-dimensional contractible manifold, rather than something more general such as an orbifold or a stratified union of manifolds. For technical simplicity, we shall assume throughout this article that \mathcal{T} is a manifold. Our results remain valid in the more general case but in that case one must work on stratified spaces (see Fischer (1970) for results on the structure of orbit spaces when they are not manifolds).

For higher-dimensional manifolds there is no analog of the Thurston geometrization program. Indeed, it is known that the set of closed n -manifolds for $n \geq 4$ is so rich that no purely algebraic classification is possible. Nevertheless, for manifolds of negative Yamabe type, every Riemannian metric g is still uniquely conformal to a metric $\gamma \in \mathcal{M}_{-1}$ so that the orbit space $\mathcal{T} = \mathcal{M}_{-1}/\mathcal{D}_0$ still represents the Teichmüller space of conformal equivalence classes on M . However, in these higher-dimensional cases, very little is known about the structure of \mathcal{T} .

The Field Equations

Relative to a global time coordinate $t = x^0$ and local spatial coordinates (x^1, \dots, x^n) on a connected closed oriented n -manifold M , one can express the line element of an arbitrary $(n+1)$ -Lorentzian metric with signature $(-\dots+)$ (n positive signs) in the form

$$ds^2 = {}^{(n+1)}g_{\mu\nu} dx^\mu dx^\nu = -N^2 dt^2 + g_{ij} (dx^i + X^i dt)(dx^j + X^j dt) \quad [5]$$

where ${}^{(n+1)}g_{\mu\nu}$ denotes the components of the space-time metric, $0 \leq \mu, \nu \leq n$, where the Riemannian metric g with components g_{ij} is the first fundamental form induced on each $t = \text{constant}$ hypersurface, where the time-dependent positive function $N = N(x, t) > 0$ is referred to as the lapse function, and where the time-dependent spatial vector field $X = X(x, t)$ with components $X^i = {}^{(n+1)}g_{0j} g^{ij}$, where g^{ij} denotes the inverse of the spatial metric g_{ij} , is referred to as the shift vector field.

Let ℓ denote the dimension *length*. In this article we use the convention that the spatial coordinates (x^1, \dots, x^n) are always dimensionless, but the time coordinate t may have a dimension (see [19] and [36]). Since the line element ds^2 [5] has dimension ℓ^2 and the spatial coordinates are dimensionless, the physical spatial metric coefficients g_{ij} also have dimension ℓ^2 . If the time coordinate t has a dimension, then the dimension of the lapse function N is such that the quantity Ndt has dimension ℓ and the dimension of the shift vector field X is such that the quantity Xdt is dimensionless.

We now briefly consider the canonical formulation of Einstein's equations. For more information regarding this formulation, see Arnowitt, Deser, and Misner (1962) (ADM) or Fischer and Marsden (1972) for a global perspective. We remark that the canonical formulation of gravity itself is local and is valid for any spatial topology of M . However, as we shall see, Hamiltonian reduction of gravity along the lines described in this article requires the topological restriction that M be of negative Yamabe type.

The standard definition of the second fundamental form k , or extrinsic curvature, induced on a $t = \text{constant}$ hypersurface leads to the coordinate formula

$$k_{ij} = -\frac{1}{2N} \left(\frac{\partial g_{ij}}{\partial t} - X_{ij} - X_{ji} \right) \quad [6]$$

where the vertical bar signifies covariant differentiation with respect to the spatial metric g and spatial indices are raised and lowered using this metric. The

natural momentum variable conjugate to g turns out to be the 2-contravariant symmetric tensor density π (that is, π is a relative tensor of weight 1) whose components in a positively oriented local coordinate chart (x^1, \dots, x^n) , that is, in a chart in the orientation atlas of M , are given by

$$\pi^{ij} = -\sqrt{\det g_{kl}}(k^{ij} - (\text{tr}_g k)g^{ij}) \quad [7]$$

where $k^{ij} = g^{ik}g^{jl}k_{kl}$ is the contravariant form of k , and where

$$\tau = \tau(g, k) = \text{tr}_g k = g^{ij}k_{ij} \quad [8]$$

is the trace of the second fundamental form, or the mean (extrinsic) curvature. From the coordinate formula [6] for the extrinsic curvature, we see that the components k_{ij} have dimension $\ell^{-1}\ell^2 = \ell$ and thus the mean curvature $\tau = \text{tr}_g k = g^{ij}k_{ij}$ has the dimension $\ell^{-2}\ell = \ell^{-1}$.

Let $\sqrt{\det g}$ denote the (global) scalar density and $d\mu_g$ denote the (global) Riemannian measure on M determined by the Riemannian metric g (note that here d is not the exterior derivative). Similarly, let μ_g denote the volume element, a nonvanishing n -form on M , determined by g and the orientation on M . In a positively oriented local coordinate chart $(x^i) = (x^1, \dots, x^n)$ on M , $(\sqrt{\det g})_{(x^i)} = \sqrt{\det g_{ij}}$, $(d\mu_g)_{(x^i)} = \sqrt{\det g_{ij}}dx^1 dx^2 \dots dx^n = \sqrt{\det g_{ij}}d^n x$, where $d^n x = dx^1 dx^2 \dots dx^n$ is the Lebesgue measure in \mathbb{R}^n , and $(\mu_g)_{(x^i)} = \sqrt{\det g_{ij}}dx^1 \wedge dx^2 \wedge \dots \wedge dx^n$. We adopt the convention of suppressing the coordinate-chart designation (x^i) so that one can, for example, write with some ambiguity $\sqrt{\det g} = (\sqrt{\det g})_{(x^i)} = \sqrt{\det g_{ij}}$.

We let

$$\text{vol}(M, g) = \int_M \mu_g = \int_M d\mu_g = \int_M \sqrt{\det g} d^n x \quad [9]$$

denote the volume of the Riemannian manifold (M, g) , given by either the integral of the volume n -form μ_g or the Riemannian measure $d\mu_g$ over M , which is given in the last integral in its coordinate form using the suppressed coordinate-chart convention adopted above. As expected, the spatial physical volume has dimension $(\ell^2)^{n/2} = \ell^n$.

We shall refer to the canonical variables (g_{ij}, π^{ij}) as the physical variables, in contrast to the reduced or conformal variables $(\gamma_{ij}, (p^{\text{TT}})^{ij})$ to be introduced later.

Note that the mean curvature $\tau = \text{tr}_g k$ is a scalar function on M whereas $\text{tr}_g \pi$ is a scalar density on M . Taking the trace of [7] expresses the mean curvature in terms of the canonical variables (g, π) ,

$$\tau = \tau(g, \pi) = \text{tr}_g k = \frac{1}{(n-1)\sqrt{\det g}} \text{tr}_g \pi \quad [10]$$

Using [10], eqn [7] can be inverted to give k in terms of g and π ,

$$k_{ij} = -\frac{1}{\sqrt{\det g}} \left(\pi_{ij} - \frac{1}{(n-1)} (\text{tr}_g \pi) g_{ij} \right) \quad [11]$$

and then combined with [6] to give the kinematical equation

$$\begin{aligned} \frac{\partial g_{ij}}{\partial t} = & \frac{2N}{\sqrt{\det g}} \left(\pi_{ij} - \frac{1}{(n-1)} (\text{tr}_g \pi) g_{ij} \right) \\ & + X_{ij} + X_{ji} \end{aligned} \quad [12]$$

In terms of the canonical variables (g, π) , a Hamiltonian form for the action for Einstein's vacuum field equations can be expressed as

$$\begin{aligned} I_{\text{ADM}}(g, \pi) = & \int_I dt \int_M \left(\pi^{ij} \frac{\partial g_{ij}}{\partial t} - N \mathcal{H}(g, \pi) \right. \\ & \left. - X^i \mathcal{J}_i(g, \pi) \right) d^n x \end{aligned} \quad [13]$$

where $I = [t_0, t_1] \subset \mathbb{R}$ is a closed interval and where the Hamiltonian (scalar) density $\mathcal{H}(g, \pi)$ and the momentum (1-form) density $\mathcal{J}(g, \pi)$ are given by

$$\begin{aligned} \mathcal{H}(g, \pi) = & \frac{1}{\sqrt{\det g}} \left(\pi \cdot \pi - \frac{1}{n-1} (\text{tr}_g \pi)^2 \right) \\ & - \sqrt{\det g} R(g) \end{aligned} \quad [14]$$

$$\begin{aligned} = & \frac{1}{\sqrt{\det g}} \left(g_{ij} g_{kl} \pi^{ik} \pi^{jl} - \frac{1}{n-1} (g_{ij} \pi^{ij})^2 \right) \\ & - \sqrt{\det g} R(g) \end{aligned} \quad [15]$$

$$\mathcal{J}_i(g, \pi) = 2(\delta_g \pi)_i = -2g_{ij} \pi^{jk}{}_{|k} \quad [16]$$

where $\pi \cdot \pi$ is the g -metric contraction of π with itself, and where, as above, $R(g)$ is the scalar curvature of the spatial metric. We also note that each of the three terms in the integrand of [13] are global scalar densities and thus can be integrated over M without any further involvement of the metric g .

Variation of I_{ADM} with respect to the lapse function and shift vector field yields the constraint equations

$$\mathcal{H}(g, \pi) = 0 \quad [17]$$

$$\mathcal{J}_i(g, \pi) = 0 \quad [18]$$

which comprise that subset of the empty space $(n+1)$ -Einstein field equations corresponding to the normal-normal and normal-tangential projections of the Einstein tensor relative to a $t = \text{constant}$ initial hypersurface. Variation of I_{ADM} with respect to π^{ij} reproduces the kinematical equation [12], whereas

variation of I_{ADM} with respect to g_{ij} generates the complementary tangential-tangential projections of Einstein's equations.

There are no evolution or constraint equations for either the lapse function N or the shift vector field X and therefore these quantities must be fixed by either externally imposed or implicitly defined gauge conditions. A convenient choice, for which a local existence and well-posedness theorem for the corresponding field equations can be established in any dimension $n \geq 2$, is given indirectly by imposing constancy of the mean curvature and a spatial harmonic gauge condition on each $t = \text{constant}$ slice (see Andersson and Moncrief (2003, 2004)). These constant mean curvature spatial harmonic (CMCSH) gauge conditions are given, respectively, by the equations

$$t = \tau \quad [19]$$

$$g^{ij}(\Gamma_{ij}^k(g) - \Gamma_{ij}^k(\hat{g})) = 0 \quad [20]$$

where from [10], τ is a function of the canonical variables (g, π) and where \hat{g} is some convenient fixed spatial reference metric (or background metric) on M . The latter condition corresponds to the requirement that the identity map between the Riemannian manifolds (M, g) and (M, \hat{g}) be harmonic. Neither of these conditions involves the lapse function or shift vector field directly but their preservation in time implemented by the demand that the time derivatives of the given conditions be enforced leads immediately to a linear elliptic system for (N, X^i) which determines these variables. The foregoing formalism is easily extended to the nonvacuum field equations in the presence of suitable material sources whose field equations are amenable to a constrained Hamiltonian treatment. To simplify the analysis, such sources will be ignored in the present discussion.

For the special case of Einstein gravity in $(2+1)$ dimensions, there is an elegant, alternative, triad-based formulation of the action functional as an $\text{Isom}(\mathbf{R}_1^3)$ -invariant gauge-theoretic Chern-Simons action, where $\text{Isom}(\mathbf{R}_1^3)$ denotes the full isometry group, or the Poincaré group (= the inhomogeneous Lorentz group), of $(2+1)$ -Minkowski space \mathbf{R}_1^3 . For nondegenerate triads the resulting field equations for this alternative formulation can easily be shown to be equivalent to those of the conventional formalism when the latter is re-expressed in terms of triads but the new formulation allows for meaningful field equations in the case of degenerate triads as well and thus suggests a potentially interesting generalization of the theory (see Carlip (1998) for details).

In any dimension $n \geq 2$, there is a well-known technique, pioneered by Lichnerowicz (1955), for

solving the constraint equations on a constant mean curvature (CMC) hypersurface (see Choquet-Bruhat and York (1980) and Isenberg (1995)). Of major importance for the treatment of Hamiltonian reduction is that if $n=2$ and $M = \Sigma_p^2$, $p \geq 2$, or if $n \geq 3$ and M is of negative Yamabe type, then every Riemannian metric g on M is uniquely globally pointwise conformal to a metric γ which satisfies $R(\gamma) = -1$ (see remark above [2]). Thus, from now on, we assume this topological condition on M . In this case, every Riemannian metric g on M can be uniquely expressed as

$$g = \begin{cases} e^{2\varphi}\gamma & \text{if } n=2 \text{ and } M = \Sigma_p^2, p \geq 2 \\ \varphi^{4/(n-2)}\gamma & \text{if } n \geq 3 \text{ and } M \text{ is of} \\ & \text{negative Yamabe type} \end{cases} \quad [21]$$

with the conformal metric γ normalized so that $R(\gamma) = -1$ and with the specific form of the coefficient conformal factor being chosen to simplify calculations involving the curvature tensors. In the case $n \geq 3$, φ is positive and thus the space of all Riemannian metrics on M is parametrized by \mathcal{M}_{-1} and the space of scalar functions $\varphi > 0$ on M . The function φ is then determined by solving the Hamiltonian constraint [17] (see also the remark before [33]).

In the given CMC slicing and imposing the vacuum field equations, since by the momentum constraint π must have zero divergence (see [16] and [18]), one finds that π^{ij} must be expressible in the form

$$\pi^{ij} = (\pi^{\text{TT}})^{ij} + \frac{1}{n}(\text{tr}_g \pi)g^{ij} \quad [22]$$

where π^{TT} is transverse (i.e., divergence-free) and traceless with respect to g . In the nonvacuum case, π^{ij} picks up an additional summand determined by the sources in the modified momentum constraint [18].

Substitution of the foregoing decompositions of (g_{ij}, π^{ij}) into the Hamiltonian constraint leads to a nonlinear elliptic equation for φ which, under the conditions assumed here, determines this function uniquely, provided $\tau \neq 0$. No solutions exist for $\tau = 0$ (equivalently, $\text{tr}_g \pi = 0$) since from [14], [17], and [22], the Hamiltonian constraint would then immediately imply that

$$R(g) = \frac{1}{\det g}(\pi \cdot \pi) = \frac{1}{\det g}(\pi^{\text{TT}} \cdot \pi^{\text{TT}}) \geq 0 \quad [23]$$

everywhere on M , which is not possible for a manifold M of negative Yamabe type. Instantaneous vanishing of the mean curvature, the defining property of a maximal hypersurface, would correspond to a moment at which an expanding universe

ceases to expand or a collapsing universe ceases to collapse. From [23], such behavior is topologically excluded here by the requirement that M be of negative Yamabe type (see also the discussion after [36]).

In the unreduced formalism of I_{ADM} , the role of a super-Hamiltonian is played by the functional

$$H_{\text{super}}(g, \pi) = \int_M (N\mathcal{H}(g, \pi) + X^i \mathcal{J}_i(g, \pi)) d^n x \quad [24]$$

which evidently vanishes whenever the constraints are satisfied. To achieve a fully reduced formulation wherein again the effective Hamiltonian would vanish, one could endeavor to solve the associated Hamilton–Jacobi equations

$$\mathcal{H}(g_{ij}, \delta S / \delta g_{ij}) = 0 \quad [25]$$

$$\mathcal{J}_k(g_{ij}, \delta S / \delta g_{ij}) = 0 \quad [26]$$

for a real-valued functional $S = S(g, \alpha^A)$ of the metric g and a set of additional independent parameters α^A . A complete solution $S(g_{ij}, \alpha^A)$ would be one for which an arbitrary solution (g_{ij}, π^{ij}) of the constraints could be realized as $(g_{ij}, \delta S / \delta g_{ij})$ for a suitable (unique) choice of the α^A . A complementary set of reduced canonical variables β_A (the momenta conjugate to the α_A 's) could then be defined by $\beta_A = \delta S / \delta \alpha^A$ and one could in principle solve the equations

$$\pi^{ij} = \frac{\delta S}{\delta g_{ij}} \quad [27]$$

$$\beta_A = \frac{\delta S}{\delta \alpha^A} \quad [28]$$

for (α^A, β_A) as functionals of the canonical variables (g_{ij}, π^{ij}) . This procedure, if it could be carried out, would ensure that these functionals $(\alpha^A(g, \pi), \beta_A(g, \pi))$ Poisson-commute with all of the constraints and hence are conserved for an arbitrary slicing of spacetime. Conversely, if a suitable set of gauge conditions such as the CMCSH conditions were imposed, one could in principle solve for the remaining independent canonical variables as functionals of the (α^A, β_A) and an internal variable, such as the mean curvature τ , which plays the role of time, and hence solve the field equations for (g_{ij}, π^{ij}) in the chosen gauge.

This proposal is purely heuristic in $(3+1)$ and higher dimensions in that there is no known procedure for finding the needed complete solution of the Hamilton–Jacobi equations in these cases. However, by exploiting the Chern–Simons analogy discussed earlier in this section, a complete solution can be found in $(2+1)$ dimensions and the corresponding complete set of “observables”

(α^A, β_A) identified. The latter are equivalent, up to a diffeomorphism of the associated reduced phase space, to a complete set of traces of holonomies of the flat $\text{Isom}(\mathbb{R}_1^3)$ -connections defined in this Chern–Simons formulation (see Carlip (1998) for more details).

The Reduced Hamiltonian

We continue with the assumption that M is a connected closed oriented n -manifold, with either $n=2$ and $M=\Sigma_p^2, p \geq 2$, or $n \geq 3$ and M of negative Yamabe type. We now define the reduced phase space as the set of conformal variables given by

$$P_{\text{reduced}} = \{(\gamma, p^{\text{TT}}) \mid \gamma \in \mathcal{M}_{-1} \text{ and } p^{\text{TT}} \text{ is a } 2\text{-contravariant symmetric tensor density that is transverse and traceless with respect to } \gamma\} \quad [29]$$

We remark that the fully reduced phase space is given by $P_{\text{reduced}}/\mathcal{D}_0$, where \mathcal{D}_0 is the group of diffeomorphisms of M isotopic to the identity. However, here, for clarity of exposition, we work on P_{reduced} rather than the fully reduced phase space.

Given a scalar function φ , with $\varphi > 0$ if $n \geq 3$, the physical variables (g, π^{TT}) are related to the conformal variables (γ, p^{TT}) by

$$(g, \pi^{\text{TT}}) = \begin{cases} (e^{2\varphi}\gamma, e^{-2\varphi}p^{\text{TT}}) & \text{if } n=2 \\ (\varphi^{4/(n-2)}\gamma, \varphi^{-4/(n-2)}p^{\text{TT}}) & \text{if } n \geq 3 \end{cases} \quad [30]$$

We adopt the convention that raising and lowering of indices on either momentum variable π^{TT} or p^{TT} will be with respect to its own conjugate metric, either g or γ , respectively. With this convention, the mixed forms of π^{TT} and p^{TT} are equal, since for $n \geq 3$,

$$(\pi^{\text{TT}})^i_j = g_{jl}\pi^{\text{TT}il} = \varphi^{4/(n-2)}\gamma_{jl}\varphi^{-4/(n-2)}p^{\text{TT}il} = \gamma_{jl}p^{\text{TT}il} = (p^{\text{TT}})^i_j \quad [31]$$

(and similarly for the $n=2$ case). Thus the squared norms of p^{TT} and π^{TT} are equal,

$$p^{\text{TT}} \cdot p^{\text{TT}} = \gamma_{ik}\gamma_{jl}p^{\text{TT}ij}p^{\text{TT}kl} = g_{ik}g_{jl}\pi^{\text{TT}ij}\pi^{\text{TT}kl} = \pi^{\text{TT}} \cdot \pi^{\text{TT}} \quad [32]$$

where in the first term the center dot is γ -metric contraction and in the last term the center dot is g -metric contraction.

The uniquely determined scalar factor φ relating the physical metric g to the conformal metric γ is obtained by solving the Hamiltonian constraint

equation [17]. In the special case that $p^{\text{TT}} = 0$ (or equivalently, from [30], that $\pi^{\text{TT}} = 0$), φ is constant and is given in the $n \geq 3$ case by

$$\varphi = \left(\frac{n}{(n-1)\tau^2} \right)^{(n-2)/4} \quad [33]$$

Thus in this case

$$\gamma = \varphi^{-4/(n-2)} g = \frac{(n-1)}{n} \tau^2 g \quad [34]$$

In particular, since τ has the dimension ℓ^{-1} (see the remark after [8]) and the components g_{ij} have the dimension ℓ^2 , we see from this formula that the conformal metric γ_{ij} is dimensionless. Although φ is not constant in the general case when $p^{\text{TT}} \neq 0$, its dimension, as in [33], is still $\ell^{(n-2)/2}$ and thus the components γ_{ij} are still dimensionless in the general case. Since in the conventions used in this article, the spatial coordinates are dimensionless, the volume $\text{vol}(M, \gamma)$ of the Riemannian manifold (M, γ) , as well as all curvature tensors of γ , are also dimensionless. Having a dimensionless conformal metric γ with a dimensionless volume has its advantages over the physical metric g with dimension ℓ^2 inasmuch, as we shall see below, an infimum of the volume of the conformal metric is related to a dimensionless topological invariant of M (see [48] and the remark thereafter).

If one now uses the conformal variables given by [30] and the decomposition [22] in the ADM action given by [13], one finds the reduced action to be

$$I_{\text{reduced}} = \int_I dt \int_M \left(p^{\text{TT}ij} \frac{\partial \gamma_{ij}}{\partial t} - \frac{2(n-1)}{n} \frac{\partial \tau}{\partial t} \sqrt{\det g} + \frac{2}{n} \frac{\partial \text{tr}_g \pi}{\partial t} \right) d^n x \quad [35]$$

In this expression one can discard the final time derivative which contributes only a boundary integral and so does not contribute to the equations of motion. Moreover, the conformal metric γ_{ij} is constrained to lie in the intersection of \mathcal{M}_{-1} and a slice for the action of \mathcal{D}_0 on \mathcal{M}_{-1} . This space can be regarded as a local chart for the reduced configuration space $\mathcal{T} = \mathcal{M}_{-1}/\mathcal{D}_0$, under the technical assumption that \mathcal{T} is a manifold. Thus, taken together, the conformal variables $(\gamma_{ij}, p^{\text{TT}ij})$ can be viewed as local canonical coordinates for the cotangent bundle $T^*\mathcal{T}$ of Teichmüller space \mathcal{T} , where $T^*\mathcal{T}$ now plays the role of the reduced phase space.

For $n=2$, these constructions can be carried out globally for the Teichmüller space \mathcal{T}_p of an arbitrary closed oriented surface Σ_p^2 , $p \geq 2$ (see the remarks after [4]). Using these global constructions, the

reduced phase space $T^*\mathcal{T}_p$ for the $(2+1)$ -reduced Einstein equations can be modeled explicitly.

Having restricted the slices to be CMC, one need only choose the relationship between the time coordinate and the CMC τ in order to fix a corresponding reduced Hamiltonian. The most natural choice of time coordinate from the present point of view is to take

$$t = t(\tau) = \frac{2}{n(-\tau)^{n-1}} \quad [36]$$

Note that this choice of time coordinate, although also denoted t , is no longer dimensionless but has dimension ℓ^{n-1} .

This choice of time coordinate is motivated by three considerations. Firstly, we remark that since $\tau=0$ is excluded in the setting used in this article (see [23] and the discussion after), τ can range in either the domain $\mathbf{R}^- = (-\infty, 0)$ or $\mathbf{R}^+ = (0, \infty)$. The usual convention on the sign of k , as adopted here, is that the sign of k is negative when the tips of the normals on a spacelike hypersurface are further apart than their bases, as for example in the expansion of a model universe, in which case $\tau = \text{tr}_g k < 0$. Thus, with this convention, τ in the range \mathbf{R}^- corresponds to an expanding universe and τ in the range \mathbf{R}^+ corresponds to a collapsing one in the future direction of increasing t . Thus for manifolds of negative Yamabe type that we consider here, the expected maximal range of the CMC τ is \mathbf{R}^- for which $\tau \rightarrow -\infty$ corresponds to a “crushing singular” big bang of vanishing spatial volume and $\tau \rightarrow 0^-$ corresponds to the limit of infinite volume expansion. Then, with the time function given by [36], the coordinate time t ranges in the interval \mathbf{R}^+ , vanishes at the big bang, and tends to positive infinity in the limit of infinite cosmological expansion.

We remark that to prove that a solution determined by Cauchy data prescribed at some initial coordinate time $t_0 \in \mathbf{R}^+$ actually exhausts the range \mathbf{R}^+ is a difficult global existence problem that is not dealt with here. Nevertheless, one of the main motivations for this work is the hope that Hamiltonian reduction will lead to advances in the study of the global existence question for Einstein's equations.

We also remark that with the choice of temporal gauge function given by [36] and with τ in its natural range \mathbf{R}^- ,

$$\frac{d\tau}{dt} = \frac{n}{2(n-1)} (-\tau)^n > 0 \quad [37]$$

so that this temporal coordinate choice preserves the time orientation of the flow for all $n \geq 2$.

Secondly, with this choice of temporal gauge, the reduced action given by [35] simplifies to

$$I_{\text{reduced}} = \int_I dt \int_M \left(p^{\text{TT}ij} \frac{\partial \gamma_{ij}}{\partial t} - (-\tau)^n \sqrt{\det g} \right) d^n x \quad [38]$$

from which one can read off an effective reduced Hamiltonian density,

$$\mathcal{H}_{\text{reduced}}(\tau, \gamma, p^{\text{TT}}) = (-\tau)^n \sqrt{\det g} \quad [39]$$

and an effective reduced Hamiltonian,

$$\begin{aligned} H_{\text{reduced}}(\tau, \gamma, p^{\text{TT}}) &= \int_M (-\tau)^n \sqrt{\det g} d^n x \\ &= (-\tau)^n \int_M d\mu_g \\ &= (-\tau)^n \text{vol}(M, g) \end{aligned} \quad [40]$$

where $\text{vol}(M, g) = \int_M d\mu_g$ is the volume of the Riemannian manifold (M, g) . Thus in terms of the physical variables (g_{ij}, π^{ij}) , the reduced Hamiltonian H_{reduced} at “time” τ is simply the volume of the CMC slice with mean curvature τ rescaled by the factor $(-\tau)^n$. With this reduced Hamiltonian density, the reduced action [38] takes the canonical form

$$I_{\text{reduced}} = \int_I dt \int_M \left(p^{\text{TT}ij} \frac{\partial \gamma_{ij}}{\partial t} - \mathcal{H}_{\text{reduced}} \right) d^n x \quad [41]$$

As the third consideration for the given choice of the time function, we note that rescaling the physical volume $\text{vol}(M, g)$ by the factor $(-\tau)^n$ yields a dimensionless quantity. Indeed, as we have seen, the spatial physical volume has the dimension ℓ^n and the constant mean curvature τ has the dimension ℓ^{-1} , so that the reduced Hamiltonian $(-\tau)^n \text{vol}(M, g)$ is dimensionless.

The main advantage of having a dimensionless reduced Hamiltonian is that only such a reduced Hamiltonian can have a topological significance, and indeed, the infimum of H_{reduced} is closely related to a dimensionless topological invariant of M (see the remarks after [48]).

In terms of the conformal variables (γ, p^{TT}) , the reduced Hamiltonian is found from [21] and [40] to be given for $n \geq 3$ by

$$\begin{aligned} H_{\text{reduced}}(\tau, \gamma, p^{\text{TT}}) &= (-\tau)^n \int_M \sqrt{\det g} d^n x \\ &= (-\tau)^n \int_M \sqrt{\det(\varphi^{4/(n-2)} \gamma)} d^n x \\ &= (-\tau)^n \int_M (\varphi^{4/(n-2)})^{n/2} \sqrt{\det \gamma} d^n x \\ &= (-\tau)^n \int_M \varphi^{2n/(n-2)} d\mu_\gamma \end{aligned} \quad [42]$$

where $d\mu_\gamma$ is the Riemannian measure on M determined by γ (locally, $d\mu_\gamma = \sqrt{\det \gamma} d^n x$) and $\varphi = \varphi(\tau, \gamma, p^{\text{TT}})$ is the conformal factor which, through the solution of the Hamiltonian constraint [17], is expressed as a function of the “time” τ and the independent conformal (or canonical) variables (γ, p^{TT}) .

In the special case $n=2, M=\Sigma_p^2, p \geq 2$, a simple formula for H_{reduced} can be derived. In terms of the conformal variables (γ, p^{TT}) , we find from [40], [10], [14], [17], [21], [22], and [32] that

$$\begin{aligned} H_{\text{reduced}}(\tau, \gamma, p^{\text{TT}}) &= \int_{\Sigma_p^2} (-\tau)^2 d\mu_g = 2 \int_{\Sigma_p^2} ((\det g)^{-1} (\pi^{\text{TT}} \cdot \pi^{\text{TT}}) - R(g)) d\mu_g \\ &= 2 \int_{\Sigma_p^2} (\det(e^{2\varphi} \gamma))^{-1} (p^{\text{TT}} \cdot p^{\text{TT}}) d\mu_{(e^{2\varphi} \gamma)} - 2 \int_{\Sigma_p^2} R(g) d\mu_g \\ &= 2 \int_{\Sigma_p^2} (e^{2\varphi})^{-2} (\det \gamma)^{-1} (p^{\text{TT}} \cdot p^{\text{TT}}) e^{2\varphi} d\mu_\gamma - 8\pi \chi(\Sigma_p^2) \\ &= 2 \int_{\Sigma_p^2} e^{-2\varphi} (\det \gamma)^{-1} (p^{\text{TT}} \cdot p^{\text{TT}}) d\mu_\gamma + 16\pi(p-1) \end{aligned} \quad [43]$$

where $\varphi = \varphi(\tau, \gamma, p^{\text{TT}})$, $\chi(\Sigma_p^2) = 2(1-p)$ is the Euler characteristic of the genus p surface Σ_p^2 , and where we have used the Gauss–Bonnet theorem

$$\int_{\Sigma_p^2} R(g) d\mu_g = 4\pi \chi(\Sigma_p^2) = 8\pi(1-p) \quad [44]$$

Since

$$\begin{aligned} H_{\text{reduced}}(\tau, \gamma, p^{\text{TT}}) &= 2 \int_{\Sigma_p^2} e^{-2\varphi} (\det \gamma)^{-1} (p^{\text{TT}} \cdot p^{\text{TT}}) d\mu_\gamma \\ &\quad + 16\pi(p-1) \geq 16\pi(p-1) \end{aligned} \quad [45]$$

the infimum of H_{reduced} is attained precisely when $p^{\text{TT}}=0$ and this infimum coincides with the topological invariant $-8\pi \chi(\Sigma_p^2) = 16\pi(p-1)$, which characterizes the surface Σ_p^2 (see also [51] below). As we shall see shortly, an analogous result holds for $n \geq 3$.

A straightforward but lengthy calculation, which is valid in arbitrary dimensions, shows that the reduced Hamiltonian is strictly monotonically decreasing in the direction of cosmological expansion except for a family of continuously self-similar spacetimes for which this Hamiltonian is constant (Fischer and Moncrief 2002b). The latter solutions exist if and only if M admits a Riemannian metric $\gamma \in \mathcal{M}_{-1}$ which is an Einstein metric, that is, for which the Ricci tensor satisfies $\text{Ric}(\gamma) = -(1/n)\gamma$. Using the mean curvature as a convenient time coordinate, that is, temporarily taking $t=\tau$, the

corresponding self-similar vacuum spacetime metrics then have the line element

$$ds^2 = -\left(\frac{n}{\tau^2}\right)^2 d\tau^2 + \frac{n}{(n-1)\tau^2} \gamma_{ij} dx^i dx^j \quad [46]$$

In the case that $n=3$, the Einstein metric γ is actually hyperbolic with constant sectional curvature $K(\gamma) = -1/6$ and Ricci curvature $\text{Ric}(\gamma) = -(1/3)\gamma$. Although the conformal variables $(\gamma, p^{\text{TT}}) = (\gamma, 0)$ are static in this model, the physical variables (g, π) are not. In this case, the resulting spacetimes (which depend on the underlying topology of M) have expanding closed hyperbolic spacelike hypersurfaces where the physical volume $\text{vol}(M, g)$ “starts” at zero at the big bang and expands to infinity in the forward time direction, as befits a universe endlessly expanding from the big bang. Such a universe is depicted in Figure 1, where the genus-2 surface is used to represent a generic closed hyperbolic 3-manifold. The Bianchi and Thurston types of this model are discussed in the next section.

The line element [46] is locally isometric to the vacuum Friedmann–Lemaître–Robertson–Walker (FLRW) $k = -1$ spacetime, which is well known to be flat. Although these spatially compactified models are technically not classical FLRW spacetimes since the expanding compact hypersurfaces are not homogeneous (and thus not isotropic), they are Lorentz-covered by the FLRW $k = -1$ spacetime and thus are locally isometric to this classical spacetime.

The same result leading to [46] holds even if matter sources are allowed, provided they satisfy a suitable energy condition, in which case the corresponding reduced Hamiltonian will only be stationary in the vacuum limit and then only when the metric is of the above type; otherwise it monotonically decays. This result even has a quasilocal

generalization expressible in terms of the corresponding quasilocal reduced Hamiltonian defined for an arbitrary domain D_τ within the CMC slice $\tau = \text{constant}$ by restricting H_{reduced} in [42] to the domain D_τ , so that for $n \geq 3$,

$$\begin{aligned} H_{D_\tau}(\tau, \gamma, p^{\text{TT}}) &= (-\tau)^n \int_{D_\tau} d\mu_g \\ &= (-\tau)^n \int_{D_\tau} \varphi^{2n/(n-2)} d\mu_\gamma \end{aligned} \quad [47]$$

If D_τ is determined from its specification on some initial slice $\tau = \tau_0$, by letting the domain flow along the normal trajectories of the CMC foliation, one can then verify that H_{D_τ} is monotonically decreasing except for the vacuum solutions of self-similar type described above, in which case H_{D_τ} is constant. This result is independent of the initial domain chosen.

We remark that one cannot use the quasilocal Hamiltonian to get equations of motion (even quasilocally) since the full true Hamiltonian is nonlocal and so one gets contributions from the whole manifold.

Since the reduced Hamiltonian H_{reduced} as well as its quasilocal variant H_{D_τ} is monotonically decreasing for generic solutions of Einstein's equations, it is natural to ask what its infimum is and whether this infimum is ever attained, at least asymptotically, by solutions of the field equations. The infimum of the reduced Hamiltonian for $n \geq 3$ and for a spatial manifold M of negative Yamabe type can be characterized in terms of a certain topological invariant of M called the sigma constant $\sigma(M)$ of M . For manifolds of negative Yamabe type, this quantity can be defined in terms of the infimum of the volume of all metrics which range over the space of conformal metrics \mathcal{M}_{-1} . The precise definition leads to the formula

$$\sigma(M) = -\left(\inf_{\gamma \in \mathcal{M}_{-1}} \text{vol}(M, \gamma)\right)^{2/n} \quad [48]$$

Interestingly, this equation defines the topological invariant $\sigma(M)$ by a purely geometrical equation involving the volume functional restricted to \mathcal{M}_{-1} . We also remark that [48] is a dimensionless equation, the left-hand side being dimensionless since it is a topological invariant of M and the right-hand side being dimensionless since the conformal metric and its volume are dimensionless (see the remarks after [34]).

Although the σ -constant can be defined for all Yamabe types, [48] holds only for manifolds of negative Yamabe type. From this equation, one can conclude that for such manifolds

$$\sigma(M) \leq 0 \quad [49]$$

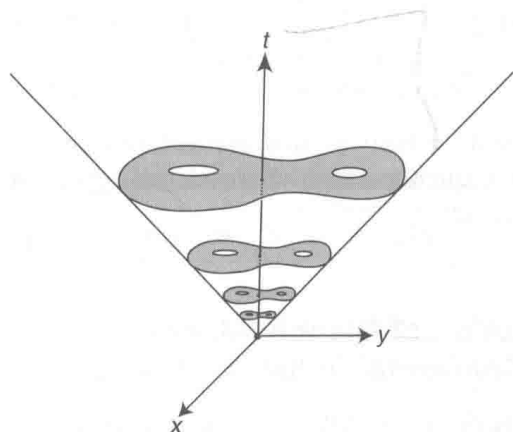


Figure 1 Expansion of the physical universe in the Bianchi V, Thurston type H^3 , spatially compactified FLRW flat spacetime cosmology.

One can relate the foregoing to the reduced Hamiltonian—by showing that the infimum of H_{reduced} defined for arbitrary $\tau < 0$ as a functional on the reduced phase space

$$T^*\mathcal{T} = T^*\left(\frac{\mathcal{M}_{-1}}{\mathcal{D}_0}\right) \quad [50]$$

is given by

$$\inf_{(\gamma, p^{\text{TT}}) \in T^*\mathcal{T}} H_{\text{reduced}}(\tau, \gamma, p^{\text{TT}}) = \begin{cases} -8\pi\chi(\Sigma_p^2) = 16\pi(p-1) & \text{if } n=2 \\ & \text{and } p \geq 2 \\ \left(\frac{n}{n-1}(-\sigma(M))\right)^{n/2} & \text{if } n \geq 3 \end{cases} \quad [51]$$

where for $n \geq 3$, M is of negative Yamabe type and thus $\sigma(M) \leq 0$ (see [49]).

One proves this result by first showing that within an arbitrary fiber of the cotangent bundle $T^*(\mathcal{M}_{-1}/\mathcal{D}_0)$, one minimizes H_{reduced} by setting the fiber variable p^{TT} to zero. In this case, the solution for the conformal factor φ reduces to a spatial constant which is a function of τ alone (see [33]), and thus the formula for H_{reduced} given in [42] reduces to

$$H_{\text{reduced}}(\tau, \gamma, 0) = \left(\frac{n}{n-1}\right)^{n/2} \text{vol}(M, \gamma) \quad [52]$$

The infimum over all conformal metrics $\gamma \in \mathcal{M}_{-1}$ of this latter functional yields the σ -constant as outlined above. If matter sources obeying a suitable energy condition are allowed, the argument goes through in much the same way with the additional implication that the infimum is achieved only for a vacuum solution so that in fact the matter must be “turned off.”

Thus, as a consequence of the above analysis, one has

$$\begin{aligned} H_{\text{reduced}}(\tau, \gamma, p^{\text{TT}}) &\geq H_{\text{reduced}}(\tau, \gamma, 0) = \left(\frac{n}{n-1}\right)^{n/2} \text{vol}(M, \gamma) \\ &\geq \left(\frac{n}{n-1}\right)^{n/2} \inf_{\gamma' \in \mathcal{M}_{-1}} \text{vol}(M, \gamma') \\ &= \left(\frac{n}{n-1}(-\sigma(M))\right)^{n/2} \end{aligned} \quad [53]$$

where the last equality follows by inverting [48] to give

$$\inf_{\gamma \in \mathcal{M}_{-1}} \text{vol}(M, \gamma) = (-\sigma(M))^{n/2} \quad [54]$$

Moreover, if $\gamma \in \mathcal{M}_{-1}$ actually achieves the σ -constant, that is, if $\text{vol}(M, \gamma) = (-\sigma(M))^{n/2}$ (and not just asymptotically approaches it as a curve or sequence), then γ must be an Einstein metric with

$$\text{Ric}(\gamma) = -\frac{1}{n}\gamma \quad [55]$$

If, additionally, $n=3$, then γ must be hyperbolic (with constant sectional curvature $K(\gamma) = -1/6$).

Although Thurston's conjectures do not refer to the σ -constant, Anderson (1997) has been able to reformulate and somewhat refine the Thurston geometrization conjectures for 3-manifolds of arbitrary Yamabe type in terms of conjectured properties of the σ -constant. Additionally, if Perelman's results are technically complete, they would provide a proof of Anderson's conjectures as well as those of Thurston's (see Anderson (2003)).

The conjectured behavior for a sequence of conformal metrics $\{\gamma_i\}$, $\gamma_i \in \mathcal{M}_{-1}$, $i=1, 2, \dots$, which seeks to minimize the volume of a stand-alone $K(\pi, 1)$ 3-manifold M of negative Yamabe type can be described as follows:

1. If M is hyperbolizable, then $\sigma(M) < 0$ is attained by a hyperbolic metric $\gamma_h \in \mathcal{M}_{-1}$, unique up to diffeomorphism, and the sequence of conformal metrics $\{\gamma_i\}$ converges to this metric in a suitable function space topology.
2. If M is a pure graph manifold, then $\sigma(M) = 0$ and the sequence $\{\gamma_i\}$ of conformal metrics “volume collapses” M with bounded curvature. Typically this occurs through collapse of circular or toroidal fibers in the associated circle or 2-torus bundle structure (see examples 3, 4, and 5 in the section “Topological Background” and see also the penultimate section). The six manifolds of flat type are not included here as they are of zero Yamabe type.
3. If M is a generic $K(\pi, 1)$ -manifold (not of type 1 or 2 above), then M can be decomposed along incompressible tori into its final finite-volume-type hyperbolizable and (possibly empty set of) graph-manifold pieces. In this case, $\sigma(M) < 0$ and the sequence $\{\gamma_i\}$ of conformal metrics collapses the graph-manifold components and converges to finite-volume complete hyperbolic metrics on the hyperbolizable components (normalized to have $R(\gamma) = -1$) yielding a σ -constant that is entirely determined by the volumes of these final hyperbolic components (see the final section).

We shall return to this conjectured characterization of sequences of conformal metrics in the next two sections.

Reduction of Bianchi Models and Conformal Volume Collapse

For manifolds of negative Yamabe type, the strict monotonic decay of H_{reduced} in the direction of cosmological expansion along nonconstant integral curves of the reduced Einstein equations suggests

that the reduced Hamiltonian is seeking to achieve its infimum $\inf H_{\text{reduced}} = ((n/(n-1))(-\sigma(M)))^{n/2}$. But does this ever happen? Does the reduced Einstein flow of the conformal geometry asymptotically approach $\inf H_{\text{reduced}}$ in the limit of infinite cosmological expansion?

To answer this question, one can consider for $n=3$ known locally homogeneous vacuum solutions of Einstein's equations which spatially compactify to manifolds of negative Yamabe type. Applying the theory of Hamiltonian reduction to these classical models, one can show that the reduced Hamiltonian behaves as expected under the reduced Einstein flow defined by these models. Since these models existed long before this theory, it is somewhat satisfying to see that they can be interpreted in terms of Hamiltonian reduction and how, with this interpretation, new properties of these classical solutions can be found.

Since H_{reduced} is a strictly monotonically decreasing function along nonconstant integral curves of the reduced Einstein flow, it is expected that under certain conditions, the reduced Hamiltonian is monotonically seeking to decay to its infimum. Thus, it is of interest to look at Hamiltonian reduction under the consequence of the following two assumptions:

1. The reduced Einstein field equations give rise to the existence of a positive semiglobal nonconstant solution $(\gamma(t), p^{\text{TT}}(t))$ defined for all $t \in (0, \infty)$ (or equivalently, for all $\tau \in (-\infty, 0)$);
2. The reduced Hamiltonian strictly monotonically decays to its infimum along nonconstant integral curves,

$$H_{\text{reduced}}(\tau(t), \gamma(t), p^{\text{TT}}(t)) \rightarrow \inf H_{\text{reduced}} \quad \text{as } t \rightarrow \infty \quad [56]$$

From [40] and [51], in terms of the physical variables (g, π) (or (g, k)), [56] can be written equivalently as

$$-\tau^3 \text{vol}(M, g) = -(\text{tr}_g k)^3 \text{vol}(M, g) \rightarrow \left(\frac{3}{2}(-\sigma(M))\right)^{3/2} \quad \text{as } t \rightarrow \infty \quad [57]$$

As a consequence of these assumptions, it follows from [53] that the conformal volume $\text{vol}(M, \gamma)$ must also decay to its infimum [54] (although not necessarily monotonically),

$$\text{vol}(M, \gamma(t)) \rightarrow \inf_{\gamma \in \mathcal{M}_{-1}} \text{vol}(M, \gamma) = (-\sigma(M))^{3/2} \quad \text{as } t \rightarrow \infty \quad [58]$$

Now suppose that $\sigma(M)=0$. A large class of manifolds for which this is true are the graph manifolds (and thus also the Seifert manifolds) of negative Yamabe type since $\sigma(M) \geq 0$ for graph manifolds in general and since $\sigma(M) \leq 0$ for manifolds of negative Yamabe type. In this case the curve $\gamma(t) \in \mathcal{M}_{-1}$ of conformal metrics must necessarily (conformally) volume collapse M in the direction of cosmological expansion,

$$\text{vol}(M, \gamma(t)) \rightarrow (-\sigma(M))^{3/2} = 0 \quad \text{as } t \rightarrow \infty \quad [59]$$

Consequently, the curve of conformal metrics $\gamma(t)$ must undergo some form of degeneration as its volume collapses. The details of this metric degeneration are of importance and are discussed below.

Not all locally homogeneous vacuum Bianchi models admit spatially compact quotients. Fortunately, the general theory of which Bianchi models admit spatially compact quotients has been worked out in detail by Tanimoto, Koike, and Hosoya (see Tanimoto *et al.* (1997) and the references therein). These Bianchi models together with their corresponding Thurston classification and typical examples of their closed quotient manifolds are listed in Table 1, where "K-S" indicates "Kantowski-Sachs," "P," "Z," and "N" denote manifolds of Yamabe type positive, zero, and negative, respectively (see the section "Topological Background"), "Seifert" means Seifert fibered, "Hyper" means hyperbolizable, "?" indicates "unknown, but conjectured to be so," and "manifold collapse" denotes the type of collapse that the conformal manifold $(M, \gamma(t))$ goes through as the conformal volume $\text{vol}(M, \gamma(t))$ collapses. We also remark that all of the manifolds

Table 1 Bianchi, Thurston, and Yamabe type of a connected closed oriented irreducible 3-manifold

Bianchi type	Thurston type	Typical examples	Yamabe type	σ -constant	Manifold structure	Manifold collapse
K-S	$S^2 \times R$	$S^2 \times S^1$	P	>0	Seifert	
IX	S^3	Nontrivial S^1 -bundles over S^2	P	>0	Seifert	
I	R^3	T^3	Z	0	Seifert	
II	Nil	Nontrivial S^1 -bundles over T^2	N	0	Seifert	Total
III	$H^2 \times R$	$\Sigma_p^2 \times S^1, p \geq 2$	N	0	Seifert	Pancake
VIII	$\text{SL}(2, R)$	Nontrivial S^1 -bundles over Σ_p^2	N	0	Seifert	Pancake
VI ₀	Sol	Nontrivial T^2 -bundles over S^1	N	0	Graph	Barrel
V, VII _h	H^3	Closed hyperbolizable manifolds	N	<0 ?	Hyper	None

listed in the "Typical examples" column are irreducible with the exception of $S^1 \times S^2$, which is prime but not irreducible. Also, in this column, $p \geq 2$.

In this table, the eight Thurston types are grouped into three sets according to their Yamabe type. The first set of such Bianchi models are those that spatially compactify to yield 3-manifolds of positive Yamabe type which allow metrics with positive constant scalar curvature, for example, Bianchi IX models defined over spherical space forms. The second set (consisting of one type) yields manifolds of zero Yamabe type which allow zero scalar curvature metrics but not constant positive scalar curvature metrics, for example, Bianchi I models defined over T^3 or one of the other five manifolds of flat type finitely covered by T^3 . The third set (the last five entries in Table 1 and the set of most interest in this article) yields manifolds of negative Yamabe type which do not allow metrics with zero scalar curvature.

These latter models are the five Bianchi models of types II, III, VIII, VI_0 , and V (and in part VII_h), which in turn correspond in Thurston's classification to manifolds of type Nil, $H^2 \times R$, $SL(2, R)$, Sol, and H^3 , respectively.

In the first three cases, the models of Bianchi type II, III, and VIII compactify to a nontrivial S^1 -bundle over T^2 or to a trivial or nontrivial S^1 -bundle over Σ_p^2 , $p \geq 2$, respectively. Each of these spaces is Seifert fibered. In the fourth case, the model of Bianchi type VI_0 compactifies to a nontrivial T^2 -bundle over S^1 which is an irreducible graph manifold. Since each of these manifolds is also of negative Yamabe type, in each of these four cases, as discussed in the beginning of this section, $\sigma(M) = 0$. In the fifth case, we consider vacuum Bianchi V metrics as well as a special case of Bianchi type VII_h which compactify to an arbitrary closed oriented hyperbolizable manifold M .

For these latter five Bianchi models that spatially compactify to manifolds of negative Yamabe type, one can consider the classical solutions from the point of view of Hamiltonian reduction. The starting point for this point of view is to use explicitly known vacuum metrics for the simplest "standard" metric forms, given, for example, in Wainwright and Ellis (1997). One need not consider all such possible spatially compact quotients, even though that would appear to be quite feasible, but one need only consider some representative examples for each of the Bianchi types listed.

It can be shown by explicit calculation, using the known solutions, that in the four nonhyperbolizable cases where $\sigma(M) = 0$, each of the classical Bianchi solutions gives rise to the existence of a positive

semiglobal nonconstant solution to the reduced Einstein field equations and that along this solution, the reduced Hamiltonian asymptotically approaches 0 under the reduced Einstein flow, thereby confirming the expectation that the reduced Hamiltonian asymptotically approaches its infimum $((3/2)(-\sigma(M)))^{3/2} = 0$. Thus in these cases the reduced Einstein flow conformally volume-collapses the 3-manifold.

The explicit calculations also show the details of this collapse. In the second and third models of Bianchi type III, Thurston type $H^2 \times R$, and Bianchi type VIII, Thurston type $SL(2, R)$, respectively, the conformal metric degenerates along embedded circular fibers and this metric degeneration causes M to collapse to its base manifold Σ_p^2 , $p \geq 2$. Since the collapse is along one-dimensional fibers and since the two-dimensional base manifold Σ_p^2 does not collapse, we refer to this type of collapse as pancake collapse (see Figure 2).

In the fourth model of Bianchi type VI_0 , Thurston type Sol, the conformal metric degenerates along embedded T^2 -fibers and this metric degeneration causes M to collapse to its base manifold S^1 . Since the collapse is along two-dimensional fibers and since the one-dimensional base manifold S^1 does not collapse, we refer to this type of collapse as barrel collapse (see Figure 3).

In the first model of Bianchi type II, Thurston type Nil, as in the second and third models, the conformal metric degenerates along embedded circular fibers. Additionally, not only do the circular fibers collapse but simultaneously the flat quotient 2-torus base manifold $T^2 \simeq M/S^1$ of M modulo its circular fibers also collapses. Thus the metric degeneration collapses M to a point, exhibiting a

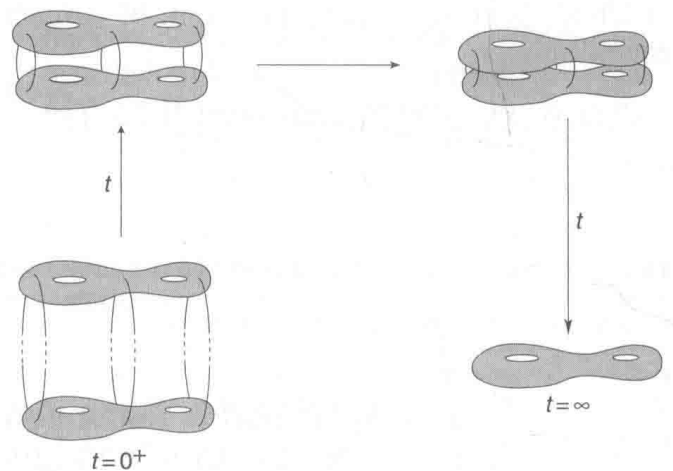


Figure 2 Bianchi III, Thurston type $H^2 \times R$, $M = \Sigma_p^2 \times S^1$, pancake collapses to Σ_p^2 , $p \geq 2$. The conformal geometry starts with an infinite S^1 -fiber at the big bang ($t = 0^+$) and pancake collapses with bounded curvature to Σ_p^2 at infinite cosmological expansion ($t \rightarrow \infty$).

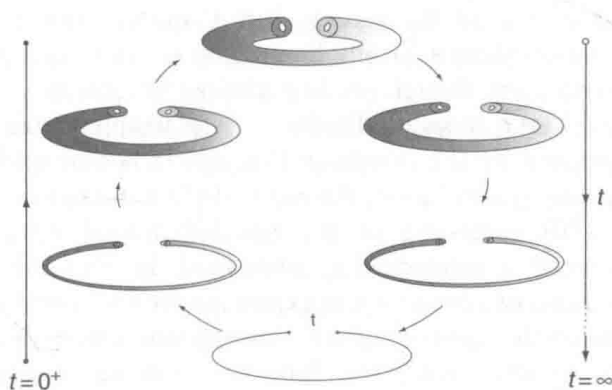


Figure 3 Bianchi VI₀, Thurston type Sol, nontrivial T^2 -bundle over S^1 , barrel collapses to S^1 . The conformal geometry evolves from a base manifold S^1 at the big bang ($t=0^+$). Instantaneously after the big bang, flat T^2 -fibers bloom out of the collapsed S^1 state. The conformal metric then expands to a maximum volume and then barrel collapses with bounded curvature back to the base manifold S^1 at infinite physical cosmological expansion ($t \rightarrow \infty$). The two facial 2-tori are flat and are glued together by an orientation-reversing toral automorphism so as to give a nontrivial T^2 -bundle over S^1 . The gray-scale density grading along the tube also indicates the nontriviality of the bundle.

case of total collapse. Thus these model universes provide examples of nonflat almost-flat manifolds that exhibit total collapse with bounded curvature. Since the conformal geometries of these model universes collapse to a point, they aptly deserve their name Nil (see Figure 4).

Remarkably, in each of these four cases of collapse, the collapse occurs with bounded curvature, precisely as occurs in the totally different setting of the Cheeger–Gromov theory of collapsing Riemannian manifolds, recognized many years ago to be of importance in the understanding of the behavior of sequences of metrics with uniform curvature bound (see Gromov (1999) for references and Anderson (2004) for other applications of Cheeger–Gromov theory to general relativity). What is somewhat remarkable is that the above cosmological models were constructed completely independently of that setting and thus provide naturally occurring cosmological models whose closed spatial hypersurfaces undergo conformal volume collapse and metric degeneration exactly as occurs in the theory of collapsing Riemannian manifolds.

Of course, this volume collapse and metric degeneration only occur as described in the conformal variables. The physical variables behave differently. Indeed, in contrast to the conformal volume which collapses to zero in the first four cases and is constant in the hyperbolizable case (see below), the volume of the physical metric in all five cases goes to infinity since the flow is

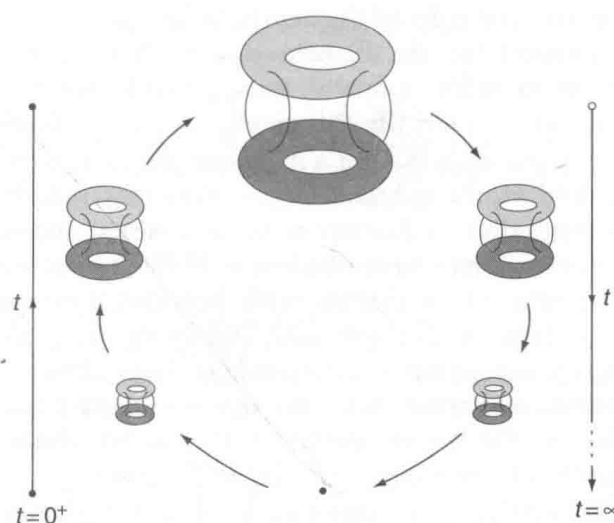


Figure 4 Bianchi II, Thurston type Nil, nontrivial S^1 -bundle over T^2 , totally collapses to a point. The conformal geometry evolves from a point at the big bang ($t=0^+$). Instantaneously after the big bang, the full 3-manifold blooms out from that point. The conformal geometry then evolves to a metric of maximum volume and then totally collapses with bounded curvature back to a point at infinite physical cosmological expansion ($t \rightarrow \infty$). The two 2-tori, represented here by doughnuts, are flat and are glued together by an orientation-reversing toral automorphism so as to give a nontrivial S^1 -bundle over T^2 .

temporally oriented in the direction of infinite cosmological expansion.

In the fifth case where M is hyperbolizable, $\sigma(M)$ is conjectured to be negative and to be determined by the hyperbolic volume, $\sigma(M) = -(\text{vol}(M, \gamma_h))^{2/3}$, of the hyperbolic conformal metric γ_h normalized so that $R(\gamma_h) = -1$. In this case, γ_h together with $p^{\text{TT}} = 0$ is a fixed point for the reduced Einstein flow so that trivially the conformal volume does not collapse. Moreover, if $\sigma(M)$ is determined by the volume of γ_h , then the constant reduced Hamiltonian also trivially achieves its infimum $H_{\text{reduced}}(\tau, \gamma_h, 0) = ((3/2)(-\sigma(M)))^{3/2} = (3/2)^{3/2} (\text{vol}(M, \gamma_h))$, again confirming the expectation for the behavior of H_{reduced} on these Bianchi models.

Note that for this static case, the physical variables behave as described after [46] and as shown in Figure 1. Also note that in contrast to Figures 2–4 where the conformal geometry is depicted, Figure 1 depicts the physical geometry.

Overall, in all five cases, subject in the hyperbolizable case to a hyperbolic metric realizing the σ -constant, the reduced Hamiltonian asymptotically approaches its σ -constant infimum along the flow lines of the reduced Einstein system. In doing so, the volumes of the conformal metrics either go to zero (in the first four cases) or to the hyperbolic volume (in the hyperbolic case). In all five cases, the curvature of the conformal metrics is uniformly bounded.

Because the reduced Einstein field equations behave as expected for the Bianchi models that we have considered with spatially compactified manifolds being either Seifert fibered, graph, or hyperbolizable, it seems plausible that for a more complicated starting manifold M , the reduced Einstein flow may induce a decomposition of M into geometric pieces. Indeed, Anderson's conjectures (Anderson 1997) predict how a sequence of geometries with bounded curvature approaching $\sigma(M)$ degenerate. Assuming these conjectures, the asymptotic behavior of large classes of Einstein spacetimes may perhaps be characterized rather explicitly in terms of the geometrization program of 3-manifolds (see the next section).

Conversely, it is conceivable that the damped hyperbolic system of equations defined by the reduced Einstein flow (with its strictly monotonically decreasing reduced Hamiltonian on nonconstant curves) could be used to try to establish some form of the geometrization conjectures for 3-manifolds, much like the parabolic system of equations defined by Ricci flow is currently being used. If such a program were to be successful, it would amount to a spectacular consequence of Einstein's equations, implying as it does that geometrization may actually occur in nature.

Possible Cosmological Applications of the Reduced Hamiltonian

Astronomical observations strongly support the view that in a sufficiently coarse-grained sense, the universe is homogeneous and isotropic. Furthermore, it is expanding at such a rate, relative to its observable energy density, that it will continue to expand forever. The simplest cosmological model consistent with these properties and which has a vacuum limit is the $k = -1$ FLRW model. Spatially compactified variants of this model are still locally homogeneous and isotropic even though they are no longer globally so (see the discussion after [46]). Evidence for one or another of the infinitely many compactifications possible could be sought in patterns of fluctuations of the cosmic microwave background radiation and the detection of such patterns could be strong evidence for a spatially closed universe.

However, is one really justified in extrapolating local observations of that portion of the universe visible to astronomers to a conclusion about its global topology? Could it be instead that there is a dynamical reason, provided by Einstein's equations, for the observed fact that the universe seems to be locally homogeneous and isotropic and in such a state as to continue expanding forever?

Suppose for the sake of argument that the universe has a more complicated topology, such as

that of one of the generic $K(\pi, 1)$ -manifolds which does not admit a locally homogeneous and isotropic metric even though its hyperbolizable components would each individually do so. A plausible scenario suggested by the results in this article is that under the Einstein evolution, the reduced Hamiltonian given by [40] consisting of the rescaled spatial volume becomes asymptotically dominated in the future direction of cosmological expansion by the contribution of the hyperbolizable components. On each of these components, the limiting conformal metric approaches local homogeneity and isotropy with the relative contribution of the graph-manifold constituents, if any are present, collapsing asymptotically to a negligible fraction of the whole. The idea is that if structure formation develops sufficiently late in the evolution of such a universe, then it should occur, with overwhelmingly high probability, in those regions which dominate the conformal volume and admit an asymptotically locally homogeneous and isotropic metric of constant negative curvature, locally indistinguishable from a $k = -1$ FLRW model.

One can speculate still further and imagine what happens if the spatial topology is not of prime type but rather consists of a connected sum of several $K(\pi, 1)$'s together perhaps with nontrivial spherical manifolds S^3/Γ and handles $S^1 \times S^2$. Here it seems conceivable, especially in view of the expected tendency of spherical manifolds to "recollapse," that the evolving universe would develop pinch-off singularities along the essential 2-spheres that separate the individual prime factors. Such singularities might occur in finite time between connected sums of spherical recollapsing factors or in infinite time between connected sums of $K(\pi, 1)$ -factors. Similar patterns of singularity formation are seen to occur in Ricci flow and must be treated in the resolution of the 3-manifold geometrization program.

Of course there is no proof of such behavior for the full $(3 + 1)$ -dimensional Einstein gravity but for the model problem of Einstein's theory in $(2 + 1)$ dimensions, something close to a proof of the analogous conjecture is already at hand. In the vacuum case, which can be described rather explicitly, one can construct the generic solution for a higher genus surface topology by cutting open the corresponding $k = -1$ FLRW model and gluing in the so-called Kazner wedges. These wedges play the role of the graph-manifold constituents of a generic $K(\pi, 1)$ -manifold in three dimensions and evolve anisotropically. However, it is known rigorously in this case that the rescaled spatial area $H_{\text{reduced}}(\tau, \gamma, p^{\text{TT}}) = (-\tau)^2 \text{Area}(\Sigma_p^2, g)$ is asymptotically exhausted by the FLRW components with the contribution from the flat Kazner anisotropic pieces shrinking to zero in this

limit. If certain types of matter sources are included, for example, those analogous to terms which result from Kaluza–Klein reduction of vacuum gravity in $(3 + 1)$ -dimensions, then a similar result can be proved at least for sufficiently small but fully nonlinear perturbations away from the vacuum backgrounds (see Choquet-Bruhat (2004)).

In fully general $(3 + 1)$ -dimensional gravity, there are few known topologically general results beyond those mentioned earlier and the problem is complicated by the presence of gravitational waves (which are absent in $(2 + 1)$ dimensions) and the fact that on such more general manifolds, there are no known “background” solutions to perturb about. However, for the special case of (future) vacuum evolution on a pure closed hyperbolizable manifold, one can show that if the initial data is sufficiently close to that of an FLRW model, then the fully nonlinear gravitational perturbations eventually die out leaving a locally homogeneous and isotropic model in the asymptotic limit (see Andersson and Moncrief (2004)). It seems likely that this result can be generalized to allow for the inclusion of various types of matter sources as in the $(2 + 1)$ -dimensional case.

Acknowledgments

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See also: Computational Methods in General Relativity: The Theory; Einstein Equations: Exact Solutions; Einstein Equations: Initial Value Formulation; Einstein Manifolds; General Relativity: Overview; Geometric Analysis and General Relativity.

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Hamiltonian Systems: Obstructions to Integrability

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Introduction

In the study of differential systems, and particularly of Hamiltonian differential equations, a fundamental problem is the question of their integrability. Because there are different definitions of this notion, a system which is integrable according to one definition can be nonintegrable according to another one. The notion of integrability is connected to the existence of a sufficiently large number of first integrals, which are linked to conservation laws. For a real analytic Hamiltonian system with n degrees of freedom, the “complete integrability” means the existence of n first integrals, which are functionally independent, and “in involution,” in the entire phase space. These integrals can be functions of class C^r (r finite), C^∞ , or analytic.

For the classical problems of Hamiltonian mechanics which are integrable, their first integrals can be continued into the complex domain of the variables, as one-valued holomorphic, or meromorphic, functions of complex time. This fact leads to the concept of “complex integrability” of a system. Note that a real Hamiltonian system which is integrable may be nonintegrable in the complex domain, if the real first integrals cannot be continued as one-valued holomorphic functions of the complex time.

Generally, the branching of solutions of a system, as functions of complex time, is an obstruction to the existence of one-valued first integrals. To study this problem, one can, following Poincaré, expand the solutions in convergent series of a small parameter: this is the base of “perturbation methods,” and the main fact is that a small perturbation of an integrable Hamiltonian system generally destroys its integrability. Another method of proving nonintegrability consists of studying the linearized equations along a particular solution. This last direction has been exploited recently, in particular, through methods based on algebraic results inspired by differential Galois theory.

Hamiltonian Systems and Mechanics

Let us consider a conservative holonomic real dynamical system with n degrees of freedom: the positions of this system are points of an

n -dimensional real manifold N (the state space or configuration space) with local coordinates x_1, x_2, \dots, x_n . If the velocities are denoted by $\dot{x}_i = dx_i/dt$, we consider the Lagrangian function L associated to this system:

$$L(x_1, \dots, x_n, \dot{x}_1, \dots, \dot{x}_n) = T(x_1, \dots, x_n, \dot{x}_1, \dots, \dot{x}_n) + V(x_1, \dots, x_n)$$

where $\dot{x} = (\dot{x}_1, \dots, \dot{x}_n)$ is a tangent vector to the manifold N at the point $x = (x_1, \dots, x_n)$. The kinetic energy $T(x, \dot{x})$ is a positive-definite quadratic form in $\dot{x}_1, \dots, \dot{x}_n$, and $V(x)$ is the potential energy, whose gradient determines the forces acting on the system.

The motions $(x_1(t), x_2(t), \dots, x_n(t))$ of the system on the manifold N are the extremals of the action integral: $\int_{t_1}^{t_2} L(x_1, \dots, x_n, \dot{x}_1, \dots, \dot{x}_n) dt$ (“principle of stationary action of Hamilton”) and they are the solutions of the Euler–Lagrange system, which consists in n differential equations of second order for the coordinates x_1, x_2, \dots, x_n (Whittaker 1904):

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}_i} \right) - \frac{\partial L}{\partial x_i} = 0, \quad 1 \leq i \leq n$$

This system can be written in the Hamiltonian form: the Lagrangian L is a function defined on the tangent bundle TN of the state space N , with local coordinates $x_1, \dots, x_n, \dot{x}_1, \dots, \dot{x}_n$ (i.e., an element of TN consists in a point x of N , joint with a tangent vector to N at x). Now, we consider the cotangent bundle T^*N : an element of T^*N consists in a point x of N joint with a cotangent vector to N at x , that is, a linear form defined in the tangent space to N at x . In local coordinates, the components of this linear form are y_1, \dots, y_n , defined by: $y_i = \partial L / \partial \dot{x}_i$; y_1, \dots, y_n are called the generalized momenta, or impulsions. x_i and y_i are called conjugate canonical variables.

The mapping from TN to T^*N thus defined is the Legendre transformation (Abraham and Marsden 1967). Through it, the Euler–Lagrange equations become a system of $2n$ differential equations of first order:

$$\frac{dx_i}{dt} = \frac{\partial H}{\partial y_i}, \quad \frac{dy_i}{dt} = -\frac{\partial H}{\partial x_i}, \quad 1 \leq i \leq n$$

where $H(x_1, \dots, x_n, y_1, \dots, y_n) = T(x_1, \dots, x_n, y_1, \dots, y_n) - V(x_1, \dots, x_n)$.

H is the Hamiltonian function of this system. The solutions of these differential equations are curves on the $2n$ -dimensional manifold T^*N , whose projections in the n -dimensional state manifold N coincide with the solutions of the Lagrangian system. T^*N is

called the phase space of the system. The second members of the differential system define a vector field in the phase space.

Let $M = T^*N$. On this $2n$ -dimensional manifold, consider the standard symplectic form $\Omega = \sum_{i=1}^n dy_i \wedge dx_i$. If f and g are C^∞ -functions on M , we define their Poisson bracket $\{f, g\}$ in local coordinates by

$$\{f, g\} = \sum_{i=1}^n \left(\frac{\partial f}{\partial x_i} \frac{\partial g}{\partial y_i} - \frac{\partial f}{\partial y_i} \frac{\partial g}{\partial x_i} \right)$$

It defines the space $C^\infty(M)$ as a Lie algebra over \mathbb{R} .

Then, if $H \in C^\infty(M)$ is the Hamiltonian function associated to a system, the corresponding Hamiltonian equations can be written as the following $2n$ "canonical equations" (Arnol'd 1976):

$$\frac{dx_i}{dt} = \{x_i, H\} = \frac{\partial H}{\partial y_i}, \quad \frac{dy_i}{dt} = \{y_i, H\} = -\frac{\partial H}{\partial x_i}, \quad 1 \leq i \leq n \quad [1]$$

A function $F \in C^\infty(M)$ is a (first) integral of eqns [1] if it is constant along any solution of [1], that is, if it verifies: $\{F, H\} = 0$. Thus, a first integral is a quantity which is preserved along a solution ("conservation law"). In particular, H itself is a first integral of the eqns [1]. It represents the "total energy" of the system.

1. The simplest example of Hamiltonian system is the harmonic oscillator defined by the one degree of freedom Hamiltonian:

$$H(x, y) = \frac{1}{2}y^2 + \frac{1}{2}x^2$$

It possesses the energy integral H . Thus, the trajectories in the phase space \mathbb{R}^2 (phase plane) are given by $x^2 + y^2 = 2h$, which are concentric circles if the constant energy verifies $h \geq 0$. The phase space \mathbb{R}^2 is foliated by these circles. The system is said to be "integrable." Obviously, it is also possible to construct Hamiltonian systems with n degrees of freedom ($n > 1$), by coupling n harmonic oscillators, with a Hamiltonian defined by

$$H(x_1, \dots, x_n, y_1, \dots, y_n) = \frac{1}{2} \sum_{i=1}^n y_i^2 + \sum_{i=1}^n a_i x_i^2$$

with n constant coefficients $a_i > 0$.

2. Another example of Hamiltonian system with one degree of freedom is the simple mathematical pendulum. The state coordinate is the angle θ of the pendulum with the vertical axis, defined modulo 2π . The phase space is: $M = S^1 \times \mathbb{R}$ ($x = \theta \pmod{2\pi} \in S^1, y \in \mathbb{R}$), that is, a cylinder. The Hamiltonian function is: $H(x, y) = (1/2)y^2 - \cos x$; H is a first integral of the differential equations, the system is integrable and the trajectories on the cylinder $S^1 \times \mathbb{R}$ are defined by

$(1/2)y^2 - \cos x = h$. According to the constant value of h on each phase curve, the solutions are periodic oscillations of the pendulum (if $h < h_0$), periodic solutions of rotation where the angle varies monotonically with time (if $h > h_0$), two equilibria (one stable, one unstable) and solutions which "begin" when $t \rightarrow -\infty$ at the unstable equilibrium and "finish" when $t \rightarrow +\infty$ at the same point (if $h = h_0$): the corresponding phase curves are called "separatrices."

3. The system of Hénon–Heiles (Hénon and Heiles 1964) is a system with two degrees of freedom. The phase space is $\mathbb{R}^2 \times \mathbb{R}^2$ and the Hamiltonian is defined by

$$H(x_1, x_2, y_1, y_2) = \frac{1}{2}(y_1^2 + y_2^2) + \frac{1}{2}(x_1^2 + x_2^2) + x_1^2 x_2 - \lambda x_2^3$$

where λ is a real constant. This system is "integrable" for some isolated values of the parameter λ (Ziglin 1983) and "nonintegrable" otherwise. Of course, it is necessary to define the integrability of a Hamiltonian system, although according to Poincaré: "A system of differential equations is only more or less integrable."

Integrability of Hamiltonian Systems

Generally, if a differential system is of order p , it is necessary to know p first integrals to integrate it. But if the system is Hamiltonian of order $2n$, only n first integrals are sufficient to integrate it "by quadratures," that is, by "algebraic" operations such as integrations and inverting of functions. The reason is that the existence of one first integral allows us to reduce the order of the system by two: a system of order $2n$ with one first integral can be reduced to order $2n - 2$.

Theorem of Liouville (see Arnol'd (1976)). Suppose that $F_1, F_2, \dots, F_n \in C^\infty(M)$ are n first integrals of the Hamiltonian system [1] which are "in involution," that is, such that: $\{F_i, F_j\} = 0, \forall i, j$, and suppose that they are functionally independent, that is, the n differentials, dF_i , are linearly independent at each point of the level set M_f defined by

$$M_f = \{(x_1, \dots, x_n, y_1, \dots, y_n) \in M : F_i(x_1, \dots, y_1, \dots) = f_i, i = 1, 2, \dots, n\}$$

Then

- (i) the set M_f is a manifold which is invariant along the solutions of the system [1];
- (ii) if M_f is compact and connected, it is diffeomorphic to an n -dimensional torus

$$T^n = S^1 \times S^1 \times \dots \times S^1 = \{(\varphi_1, \dots, \varphi_n) : \varphi_i \in \mathbb{R}/2\pi\mathbb{Z}\};$$

- (iii) the Hamiltonian flow on each torus M_f is linear and “quasiperiodic” with frequencies ω_i defined by $d\varphi_i/dt = \omega_i(f_1, f_2, \dots, f_n)$; and
- (iv) the Hamiltonian equations are integrable by quadratures.

If a Hamiltonian verifies the assumptions of the theorem of Liouville, one can prove that it exists, locally, canonical coordinates $\varphi = (\varphi_1, \dots, \varphi_n)$ and $I = (I_1, \dots, I_n)$ such that the Hamiltonian function depends only on the variables I_i . Then

$$\begin{aligned}\frac{d\varphi_i}{dt} &= \frac{\partial H}{\partial I_i} \\ \frac{dI_i}{dt} &= -\frac{\partial H}{\partial \varphi_i} = 0\end{aligned}$$

These equations are immediately integrated as follows:

$I_i = \text{constant}$, and $\varphi_i = \omega_i \cdot t + \varphi_i(0)$, with

$$\omega_i(I_1, I_2, \dots, I_n) = \left. \frac{\partial H}{\partial I_i} \right|_{I=cst}$$

Such local coordinates (φ_i, I_i) are called “action-angle” variables. They were defined for the first time by Delaunay and they play an important part in the theory of perturbations.

Remark An invariant torus T^n of the theorem of Liouville is characterized by the constant values of the actions I_i , which determine the frequencies ω_i on it. Such a torus is said to be nonresonant if the relation between the frequencies ω_i : $\sum_{i=1}^n k_i \omega_i = 0$ (where k_1, \dots, k_n are integers) implies that $k_i = 0, \forall i$. The frequencies ω_i are then rationally independent. If a torus is nonresonant, the phase trajectories are dense everywhere and the motion is quasiperiodic on it.

A torus is said to be resonant, if the frequencies ω_i are rationally dependent: they verify a relation $\sum_{i=1}^n k_i \cdot \omega_i = 0$, with $(k_1, \dots, k_n) \neq (0, \dots, 0)$. Then the phase trajectories are not dense on the torus; they belong to tori of lower dimension.

A consequence of the theorem of Liouville is that, if a two-degree-of-freedom Hamiltonian system possesses one first integral F (in addition to H , and independent of H), it is integrable because F is necessarily in involution with H : $\{F, H\} = 0$.

An example of system with three degrees of freedom which is integrable is the Lagrangian symmetric top with one fixed point (there exists a cylindric symmetry for the inertia momenta and the center of mass is on the symmetry axis). This system possesses three first integrals that are in involution and independent: H , and the angular momenta M_2 and M_3 , which correspond to the (constant)

frequencies of precession and nutation of the top. The level sets M_f are here tori of dimension 3, which are indexed by the three frequencies (or by the constant values of the three integrals).

There are other integrable cases for this problem of a rigid body with a fixed point (see Kozlov (1983)): the Euler’s case (when the fixed point is the center of mass); the Kowalevskaya’s case (in which the inertia momenta verify two relations and the third coordinate of the center of mass vanishes – see Kowalevski (1889)); and the Goryachev–Chaplygin’s case, which is integrable only on a single integral level.

A fundamental and classical example of integrable Hamiltonian system is the Kepler’s problem: the motion of a ponctual mass in the gravitational (Newtonian) field of a center, for instance, a planet in the field of attraction of the Sun.

Another example is the problem of two fixed centers: an infinitesimal mass in the field of two centers, problem which was integrated by Lagrange (Lagrange, 1810).

Isolated Periodic Orbits and Nonintegrability

We consider a real Hamiltonian system with n degrees of freedom and we suppose that there exists a particular T -periodic solution Γ_T (which is not an equilibrium). Along Γ_T , we consider the linearized equations deduced from the Hamiltonian system. They can be decoupled into the tangential equation (one degree of freedom) which possesses the first integral dH and the normal variational system which can be written as

$$\frac{d\xi}{dt} = J \cdot K(\Gamma_T(t)) \cdot \xi \quad [2]$$

where

$$J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}$$

is the standard symplectic matrix of order $2(n-1)$ and $K(\Gamma_T(t))$ is a T -periodic matrix depending on the solution Γ_T .

The solutions of the linear system [2] form a vector space. As a definition, the monodromy matrix $M(T)$ expresses how fundamental solutions of the linear system [2] are transformed after one period T , that is, along the periodic closed orbit Γ_T :

$$\xi(t+T) = M(T) \cdot \xi(t)$$

Poincaré showed that if one of the eigenvalues of $M(T)$ is different from 1, then the periodic solution Γ_T is isolated. Furthermore, if the number of first

integrals of the Hamiltonian system, independent along Γ_T , is equal to k , then at least $2k$ eigenvalues of $M(T)$ are equal to 1.

Theorem (Poincaré 1892). *If the Hamiltonian system possesses n integrals in involution, and independent along a periodic solution Γ_T , then Γ_T is nonisolated.*

Then, if the Hamiltonian system possesses a dense set of isolated periodic orbits, it cannot have n integrals in involution and independent in an open domain.

Nearly Integrable Hamiltonian Systems, Theorem of Poincaré

Consider the Hamiltonian system with n degrees of freedom, depending on a small real parameter $\varepsilon \in (-\varepsilon_0, +\varepsilon_0)$, defined by the analytic function H :

$$H(\varphi, I, \varepsilon) = H_0(I) + \varepsilon \cdot H_1(\varphi, I) \quad [3]$$

where $\varphi = (\varphi_1, \dots, \varphi_n) \in T^n$, $I = (I_1, \dots, I_n) \in \mathbb{R}^n$, and where H_1 is periodic in the angles φ_i .

This system is called “nearly integrable” because when $\varepsilon = 0$, the “unperturbed system” H_0 is integrable in the action-angle variables φ, I :

$$H(\varphi, I, 0) = H_0(I)$$

then

$$\frac{dI}{dt} = 0, \quad \frac{d\varphi}{dt} = \frac{\partial H_0}{\partial I} = \omega(I)$$

system which can be integrated by quadratures:

$$I = I^0 \quad \text{and} \quad \varphi = \varphi^0 + \omega(I^0) \cdot t$$

According to the theorem of Liouville, the motion of the unperturbed problem takes place on n -dimensional tori $(S^1)^n$ in the phase space. On these invariant tori, indexed by the actions I , the motion is generally quasiperiodic (if the frequencies $\omega(I)$ are rationally independent).

We are now interested in studying the perturbed system [3] with $\varepsilon \neq 0$, and its integrability which is, according to Poincaré (1892), “the fundamental problem of dynamics.” This problem of nearly integrable Hamiltonian systems is directly inspired by celestial mechanics where the motions in the solar system are, in a first approximation, described by the (integrable) Kepler’s problem. In particular, the “restricted three-body problem” is the study of the motion of a planet in the gravitational field of the Sun, with the perturbative attraction of Jupiter. It is also the problem of the Moon in the field of the Earth, with the perturbative attraction of the Sun (Poincaré 1892).

Theorem of Poincaré (Poincaré 1892). *Assume that, in the Hamiltonian function [3]:*

- (i) (nondegeneracy condition) *the unperturbed Hamiltonian H_0 is nondegenerate, that is,*

$$\det \left| \frac{\partial^2 H_0}{\partial I_i \partial I_j} \right| = \det \left| \frac{\partial \omega_i}{\partial I_j} \right| \neq 0$$

in an open domain of the phase space;

- (ii) (genericity condition) *no coefficient $h_k(I)$ in the Fourier expansion of H_1 with*

$$H_1(\varphi, I) = \sum_{k \in \mathbb{Z}^n} h_k(I) \cdot e^{i(k, \varphi)}$$

does identically vanish in the nonresonant domain $G \in \mathbb{R}^n$ of the actions defined by

$$G = \left\{ I \in \mathbb{R}^n : \sum_{i=1}^n k_i \cdot \omega_i(I) = 0, \right. \\ \left. \text{iff } (k_1, \dots, k_n) = (0, \dots, 0) \right\}$$

then, there is no analytic first integral $F(\varphi, I, \varepsilon)$ independent of the Hamiltonian function H .

Thus, a perturbation of a nondegenerate integrable Hamiltonian system is generically nonintegrable.

When one wants to apply this theorem to celestial mechanics, a peculiarity is that the unperturbed problem corresponds to the Keplerian system, which is degenerate, and this is a specific difficulty of these systems.

Splitting of Separatrices and Nonintegrability

Consider a Hamiltonian system with $n=2$ (degrees of freedom) defined as in eqn [3] by a perturbation of an integrable Hamiltonian:

$$H(\varphi_1, \varphi_2, I_1, I_2, \varepsilon) \\ = H_0(I_1, I_2) + \varepsilon \cdot H_1(\varphi_1, \varphi_2, I_1, I_2) \quad [4]$$

The unperturbed problem is integrable and its four-dimensional phase space is foliated by two-dimensional invariant tori $T^2 : I = \text{constant}$. If H_0 is nondegenerate, the nonresonant tori are dense and the resonant tori also are dense in the phase space.

According to Kolmogorov’s theorem and the Kolmogorov–Arnol’d–Moser (KAM) theory (Arnol’d 1985), the majority of the nonresonant tori of the unperturbed problem H_0 are preserved in the full problem [4]: they are slightly deformed, and are invariant in the perturbed

system. The resonant tori of H_0 are destroyed in the perturbed problem.

Now we consider, in the phase space, a transverse surface S to the invariant tori T^2 of the perturbed system. A trajectory of the system generated by [4], which crosses S through a point w_0 , will cross S again, for the first time, through a point w_1 : this defines the “first return map” or “Poincaré’s map” $R: w_0 \mapsto R(w_0) = w_1$. S is called a Poincaré’s section. If w_0 belongs to a preserved invariant torus of the perturbed system, the successive points $w_0, w_1 = R(w_0), w_2 = R(w_1), w_3 = R(w_2), \dots$ belong to the intersection of this torus with S ; thus, they belong to a curve diffeomorphic to a circle, which is an invariant curve of the map R . If w_0 does not belong to a preserved invariant torus of [4], the sequence of points w_0, w_1, w_2, \dots through the Poincaré’s map belongs to a curve much more complicated than a curve diffeomorphic to a circle (Poincaré 1890, Arnol’d 1985) and the “chaotic” behavior of this sequence is the mark of the nonintegrability of the system [4].

The best way of numerically showing the “evidence” of nonintegrability is to study the example of a system with “one and a half” degree of freedom, that is, a system with one degree of freedom whose Hamiltonian depends on time: $H(\varphi, I, t)$. An example of such a system is the problem of a mathematical pendulum whose length l performs periodic oscillations, defined by the Hamiltonian function

$$H(\varphi, p, t) = \frac{p^2}{2} - \omega^2(1 + \varepsilon \cdot f(t)) \cdot \cos \varphi \quad [5]$$

where $\varphi \in S^1$, $p \in \mathbb{R}$, and f is periodic of period T .

The unperturbed system ($\varepsilon = 0$) is integrable (one degree of freedom with a Hamiltonian independent of t):

$$H_0(\varphi, p) = \frac{p^2}{2} - \omega^2 \cdot \cos \varphi$$

The phase portrait of this problem is similar to the one of the simple mathematical pendulum of constant length: on the cylinder $S^1 \times \mathbb{R}$ there are two equilibria (stable and unstable) and separatrices “beginning” and “finishing” at the hyperbolic point χ . The invariant stable and unstable manifolds associated to χ and represented by these separatrices were called by Poincaré as “homoclinic” trajectories, because each of them, drawn on the phase cylinder, joins equilibrium χ to itself.

If $\varepsilon \neq 0$, we define a Poincaré section of the perturbed system [4] in the following way: from an initial point $w_0(\varphi_0, p_0, t_0)$, we consider the successive

planes perpendicular to the t -axis in the “extended” phase space $\{(\varphi, p, t)\}$, defined by: $t_0, t_1 = t_0 + T, t_2 = t_0 + 2T, t_3 = t_0 + 3T, \dots$ and we look at the successive intersections of the orbit of w_0 with these planes: w_0, w_1, w_2, \dots . If we identify all the successive planes and if we draw on the same picture, the points w_0, w_1, w_2, \dots , we obtain a phase portrait in which the equilibria of the unperturbed problem are present, but the separatrix which “leaves” the point χ is not confounded with the separatrix which “ends” at χ , as in the unperturbed problem: the two invariant curves are transversal to each other: they “split” and have an infinite number of intersections. This splitting is the traduction of the nonintegrability of the perturbed system [5].

A method to detect this splitting of separatrices consists in computing the Melnikov’s function which gives a measure of the angle between the separatrices at their first intersection when they split.

Many concrete Hamiltonian systems have been studied by this method and numerical investigations on the splitting have permitted detection of their nonintegrability.

Topological Obstructions to Integrability

We are interested in a natural mechanical system with two degrees of freedom and we suppose that the state space N is a real analytic surface which is compact and orientable. Then, N consists of a two-dimensional sphere with k handles (or a torus with k holes). The number k is a topological invariant of the surface and is called the genus of N .

Let H be the Hamiltonian function associated to this problem. The Hamiltonian system possesses the first integral H . It is completely integrable if and only if another analytic integral F exists, functionally independent of H . In this case, the state space N belongs necessarily to a very restrictive class of surfaces.

Theorem (Kozlov 1983). *If the genus k of the state manifold N is not equal to 0 or 1 (i.e., if N is neither diffeomorphic to the sphere S^2 nor to the torus T^2), then the Hamiltonian system generated by H does not possess a first integral, analytic on T^*N and functionally independent of the energy integral H .*

Note that this theorem does not apply to first integrals which are C^∞ only, and examples can be given which illustrate this case (Kozlov 1983, 1989).

For systems with more than two degrees of freedom, an open question is to know whether the complete integrability imposes restrictions to the topology of the state manifold N .

Singular Point Analysis, Branching of Solutions and Ziglin's Theory

If we look at the classical Hamiltonian problems which have been integrated, their first integrals are real functions which can be continued in the complex domain as one-valued holomorphic or meromorphic functions of the complex time t (polynomials, rational functions, etc.). This fact leads to the concept of "complex integrability." But the nonintegrability of a complex Hamiltonian system does not imply the nonintegrability of its restriction to the real domain: it may happen that a real analytic first integral does not possess a continuation in the complex domain as a meromorphic function.

Adopting this point of view, S Kowalevskaya (Kowalevski 1889) studied the problem of a top rotating around a fixed point, and she discovered a new case of integrability for this classical problem of Hamiltonian mechanics. She searched for conditions on the parameters such that the movable singularities of the solutions in the complex plane of time are poles (as a definition, a singularity is movable if its location in the complex domain depends on the initial conditions). Such differential systems are said to be of "Painlevé's type." In this case, the solutions are single valued in the complex t -plane and there is no branching of these solutions. The leading idea is the following: a first integral must be constant along a solution, and an eventual branching would change its value along a loop around a singularity in the complex t -plane. However, finite branchings of solutions can be compatible with integrability.

The main tool in this analysis is the calculation of the "Kowalevski's exponents" which determine the eventual branching of a solution around a singularity.

In spite of the efficiency of the Painlevé analysis for the search of integrable (or nonintegrable) systems, the relation between the analytic properties of their solutions (Painlevé) and their integrability in the sense of Liouville remains mysterious. The most fundamental result obtained in this field is a theorem of Adler and van Moerbeke which proves that, if a system has the Painlevé property and if it is integrable in the sense of Arnol'd-Liouville, then it is algebraically integrable (Adler and van Moerbeke 1989).

The discovery of S Kowalevskaya inspired Ziglin, who related the existence of meromorphic first integrals for a Hamiltonian system, to the properties of the linearized equations along a particular periodic solution of this system, especially to the monodromy group associated to this linear system. Ziglin used the constraints imposed

to this monodromy group by the existence of first integrals.

Let us consider a Hamiltonian system defined on a complex analytic symplectic manifold of dimension $2n$, and suppose that there exists a family of periodic solutions Γ . The linearized equations deduced from the Hamiltonian system along Γ are decoupled into tangential and normal equations. We are interested by the normal equations, which are linear with periodic coefficients.

Ziglin's Theorem (Ziglin 1983). *Assume that a Hamiltonian system has a family of particular solutions Γ_b (which are not equilibria) parametrized by periodic functions of the complex time and depending analytically on a real parameter $b \in (b_1, b_2)$. Let G be the monodromy group of the normal variational equation associated to the solution Γ_b . A monodromy matrix $g \in G$ is said to be nonresonant if every eigenvalue of g is different from a root of unity. If the Hamiltonian system has a meromorphic integral F , functionally independent of the Hamiltonian H in a neighborhood of Γ_b , and if the monodromy group G contains a nonresonant element g_1 , then for any $g_2 \in G$, the commutator $g^* = g_2^{-1} \cdot g_1^{-1} \cdot g_2 \cdot g_1$ satisfies either $g^* = \text{Id}$ or $g^* = (g_1)^2$.*

As a corollary of this theorem, we have sufficient conditions of nonintegrability: if the necessary conditions of integrability of Ziglin are not satisfied by a Hamiltonian system, it is not analytically integrable. For instance, this will happen if we can find two nonresonant monodromy matrices g_1 and g_2 which do not commute. If the periodic solution Γ_b has two complex periods, the monodromy group G has generators g_1 and g_2 , respectively associated to each of these periods and their commutativity can be sometimes studied.

These sufficient conditions of nonintegrability were studied for particular Hamiltonian systems, first by Ziglin himself.

Several concrete systems with two degrees of freedom were proved to be nonintegrable by Ito, Yoshida, Churchill, Rod, and many other mathematicians who applied this "Ziglin's method": for instance, the Hénon-Heiles system, the Yang-Mills system, and Hamiltonian systems with a homogeneous potential.

Nonintegrability and Differential Galois Theory (Morales-Ruiz 1999)

Recently, the integrability of Hamiltonian systems was studied with algebraic tools from the differential Galois theory, applied to linear differential

systems. As in Ziglin's theory, we consider a particular solution Γ (not necessarily periodic) of a differential system generated by an analytic Hamiltonian H with n degrees of freedom, and the (linear) variational equations along Γ . The idea is that, if the Hamiltonian system is integrable, we can assume that the linearized equations along Γ must also have a "regular behavior." If the Hamiltonian system is integrable, it will also be the case for the variational equations.

The normal variational system (of order $2n - 2$) can be written as

$$\frac{d\xi}{dt} = J \cdot K(\Gamma(t)) \cdot \xi \quad [6]$$

with

$$J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}$$

$K(\Gamma(t))$ is a matrix depending on the particular solution Γ .

We have to define the "Galois group" of the linear equation [6]. Recall that in the classical Galois theory of algebraic equations, the Galois group is defined by the automorphisms which map roots onto roots of the equation. In an analogous way, in the differential Galois theory, we consider the maps which send a fundamental solution of eqn [6] on a fundamental solution. In order to define the Galois group G associated to [6], we consider a differential field K of functions over C (i.e., a field of functions equipped with a derivation). The field of constants of K is C ; it is the subfield of K whose elements have a derivative equal to zero. We denote by $K\langle\xi, \eta, \dots\rangle$ the differential field extension obtained from K by the adjunction of the functions ξ, η, \dots . If (φ, ψ) is a fundamental system of solutions of eqn [6], then $L = K\langle\varphi, \psi\rangle$ is the smallest differential field extension which contains all the solutions of [6]. The field of constants of L is the same as the one of K , that is, C . By definition, L is a Picard-Vessiot extension of K .

The differential Galois group of L is defined as the group of the automorphisms γ of L (that map a solution of [6] onto a solution) leaving the field of constants fixed. Given a fundamental system of solutions (φ, ψ) , we can associate to each automorphism γ the matrix M such that $(\gamma(\varphi), \gamma(\psi)) = (\varphi, \psi) \cdot M$. By definition, the set of these matrices M is the Galois group G of eqn [6]. It is a linear algebraic group (because, the matrices M being symplectic, their coefficients verify polynomial equations) and a subgroup of the linear group of matrices $GL(C)$. We note that, for a given linear system, the monodromy group is contained in the Galois group and both are subgroups of the symplectic group $Sp(C)$.

In the Galois group G of eqn [6], we consider G^0 , the connected component of the identity. The integrability of the initial Hamiltonian system is connected to the integrability of the variational equation [6] and, through it, to the properties of its Galois group:

Theorem of Morales and Ramis (Morales-Ruiz 1999). *If an analytic Hamiltonian system is completely integrable, then the Galois group associated to the variational equation along a particular solution Γ is such that its connected component of identity G^0 is Abelian.*

Thus, if a Hamiltonian system is such that G^0 is not Abelian, there cannot exist a complete set of first integrals in involution in a neighborhood of the particular solution Γ and the system is not integrable.

In the concrete applications of this theory, an algorithm of Kovacic allows us to determine the Galois group explicitly. By this method, several Hamiltonian systems were proved to be nonintegrable: for instance, systems of points on a line with a potential in $1/r^2$, studied by Julliard-Tosel (1998), but also ancient proofs of nonintegrability of homogeneous potentials, which were improved by Yoshida and Umeno, thanks to the theorem of Morales-Ramis.

See also: Billiards in Bounded Convex Domains; Infinite-Dimensional Hamiltonian Systems; Integrable Systems: Overview; Peakons; Separatrix Splitting.

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Hamiltonian Systems: Stability and Instability Theory

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The solar system has long appeared to astronomers and mathematicians as a model of stability. On the other hand, statistical mechanics relies on the assumption that large assemblies of particles form highly unstable systems (at the microscopic scale). Yet all these physical situations are described, at least to a certain degree of approximation, by Hamiltonian systems.

One may hope that Hamiltonian systems can be classified in two different categories, stable and unstable ones. However, the situation is much more complicated and both stable and unstable behaviors cohabit in typical systems. Even our examples are not perfect paradigms of stability and instability. Indeed, it is now clear from numerical as well as theoretical points of views that some instability is present over long timescales in the solar systems, so that for example future collisions between planets cannot be completely ruled out in view of our present understanding. On the other hand, unexpected patterns of stability have been discovered in systems involving a large number of particles.

Understanding the impact of stable and unstable effects in Hamiltonian systems has been considered ever since Poincaré as one of the most important questions in dynamical systems. In this article, we will discuss model Hamiltonian systems of the form

$$H_\epsilon(q, p) = h(p) + \epsilon G_\epsilon(q, p)$$

where $(q, p) \in \mathbb{T}^d \times U$, with U a bounded open subset of \mathbb{R}^n . Recall that the equations of motion are

$$\dot{q}(t) = \partial_p h(p) + \epsilon \partial_p G_\epsilon(q, p) \quad [1]$$

$$\dot{p}(t) = -\epsilon \partial_q G_\epsilon(q, p) \quad [2]$$

The textbook by Arnol'd (1964) is a good general introduction on Hamiltonian systems. We will always denote by $\omega(p)$ the frequency map $\partial_p h(p)$, which plays a crucial role. Here, as is obvious in [2], the action variables p are preserved under the evolution in the unperturbed case $\epsilon = 0$. We will try to explain what is known on the evolution of these action variables for the perturbed system. As we will see, in many situations, these variables are extremely stable. For example, KAM theorem implies that, for a positive measure of initial conditions (q_0, p_0) the trajectory $(q(t), p(t))$ satisfies $\|p(t) - p(0)\| \leq C\epsilon$ for all times. Examples show that some initial conditions may lead

to unstable trajectories, that is, trajectories such that $\|p(t) - p(0)\| \geq 1/C$ for some t (depending on ϵ) and some fixed constant C independent of ϵ . However, this is, as we will see, possible only for very large time t (meaning that t as a function of ϵ has to go to infinity very quickly when $\epsilon \rightarrow 0$). The main questions here are to understand in what situation instability is or is not possible, and what kind of evolutions can have the action variable p . Another important question is to estimate the speed (as a function of the parameter ϵ) of the evolutions of p .

A Convention

We assume, unless otherwise stated, that the Hamiltonians are real analytic. The norm $|H|$ of the Hamiltonian H is the uniform norm of its holomorphic extension to a certain complex strip. We do not specify the width of this strip. Whenever we consider a family $H_\epsilon, F_\epsilon \dots$ of Hamiltonians, we mean that the norm $|H_\epsilon|$ is bounded when $\epsilon \rightarrow 0$.

Averaging and Exponential Stability

The first observation concerning the action variables is that they should evolve at a speed of the order of ϵ . However, averaging effects occur. More precisely, in the equation $\dot{p}(t) = -\epsilon \partial_q H_\epsilon(q(t), p(t))$, the variable $q(t)$ is moving fast compared to $p(t)$. If the evolution of $q(t)$ nicely fills the torus \mathbb{T}^d , it is tempting to think that the averaged equation

$$\dot{\bar{p}}(t) = -\epsilon \bar{V}_\epsilon(\bar{p}(t))$$

should approximate accurately the actual behavior of $p(t)$, where

$$\bar{V}_\epsilon(p) := \int_{\mathbb{T}^d} \partial_q H(q, p) dq$$

We have $\bar{V} \equiv 0$, which leads us to think that the evolution should consist mainly of oscillations of small amplitude with no large evolution. This reasoning is limited by the presence of resonances.

Frequencies

A frequency $\omega \in \mathbb{R}^d$ is said to be resonant if there exists $k \in \mathbb{Z}_*^d (= \mathbb{Z}^d - \{0\})$ such that $\langle k, \omega \rangle = 0$. The resonance module of ω ,

$$Z(\omega) = \{k \in \mathbb{Z}^d / \langle k, \omega \rangle = 0\}$$

is a subgroup \mathbb{Z}^d ; we denote by $R(\omega)$ the vector space generated by $Z(\omega)$ in \mathbb{R}^d . The order of resonance $r(\omega)$ is the dimension of $R(\omega)$. The main examples of resonances of order r are the

frequencies $\omega = (\omega_1, 0)$, where $\omega_1 \in \mathbb{R}^{d-r}$ is nonresonant. This example is universal. Indeed, if ω is a resonant frequency, then there exists a matrix $A \in \text{Gl}_d(\mathbb{Z})$ such that $A\omega = (\omega_1, 0)$, where $\omega_1 \in \mathbb{R}^{d-r}$ is not resonant. The matrix A can be seen as a diffeomorphism of \mathbb{T}^d , which transports the constant vector field ω to the constant vector field $A\omega = (\omega_1, 0)$. It is useful to distinguish, among nonresonant frequencies, some which are sufficiently nonresonant. A frequency $\omega \in \mathbb{R}^d$ is called Diophantine if there exist real constants $\gamma > 0$ and $\tau \geq d$ such that

$$|\langle \omega, k \rangle| \geq \gamma \|k\|^{1-\tau}$$

for each $k \in \mathbb{Z}_*^d$. Finally, a frequency is called resonant Diophantine if there exists a matrix $A \in \text{Gl}_n(\mathbb{Z})$ such that $\omega = A(\omega_1, 0)$, where $\omega_1 \in \mathbb{R}^{d_1}$ is a Diophantine frequency.

Symplectic Diffeomorphisms and Normal Forms

An efficient mathematical method to take averaging effects into account is the use of normal forms. Normal form theory consists in finding new coordinates in which the fast angles have been eliminated from the equations up to a small remainder. This is done exploiting the existence of a large group of diffeomorphisms preserving the Hamiltonian structure of equations, called symplectic diffeomorphisms or canonical transformations. We refer the reader to standard textbooks for these notions, for example to Arnol'd (1964). An important point is that a symplectic diffeomorphism ϕ sends the trajectories of the Hamiltonian $H \circ \phi$ to the trajectories of the Hamiltonian H . A Hamiltonian $N(q, p)$ is said to be in R -normal form, where R is a linear subspace of \mathbb{R}^n , if $\partial_q N \in R$ for each (q, p) . Let us give an illustrative result, taken from Lochak *et al.* (2003). Note that this result is not sufficient to obtain uniform stability estimates, as in Nekhoroshev theorem below. More precise normal form results are given in Nekhoroshev (1977) and Pöschel (1993).

Normal Form Theorem

Let $\omega_0 = \omega(p_0)$ be a given Diophantine or resonant-Diophantine frequency. Let us denote $B_r(p_0)$ the open ball of radius r in \mathbb{R}^d centered at p_0 . There exists a constant a which depends only on ω , and constants $\epsilon_0 > 0$ and $C > 0$ such that the following holds: for each $\epsilon < \epsilon_0$, there exists an analytic symplectic embedding $\phi_\epsilon: \mathbb{T}^d \times B_{r(\epsilon)} \rightarrow \mathbb{T}^d \times U$, which is ϵ -close to identity and such that

$$H_\epsilon \circ \phi_\epsilon(q, p) = h(p) + \epsilon N_\epsilon(q, p) + \mu(\epsilon) F_\epsilon(q, p)$$

where N is in $R(\omega_0)$ -normal form, $r(\epsilon) \geq \sqrt{\epsilon}$, and $\mu(\epsilon) \leq e^{-C\epsilon^{-a}}$.

This means that the motions with resonant initial conditions are confined, up to small oscillations, in the associated affine plane $p(0) + R(\omega(p(0)))$ until they live in the domain of the normal form, or until time $\mu^{-1}(\epsilon)$.

Geometry of Resonances

In view of the normal form theorem, we are led to consider the curves $P(\theta): \mathbb{R} \rightarrow \mathbb{R}^d$ which satisfy

$$P(\theta') - P(\theta) \in R(\omega(P(\theta)))$$

for each θ and θ' . Indeed, it appears that these curves are the ones the action variables can follow on timescales not involving the remainders of the normal forms. Note that here the parameter θ is not the physical time. Assuming that $P(\theta)$ is such a curve, we can define the affine space

$$R := P(0) + \cap_{\theta \in \mathbb{R}} R(\omega(P(\theta)))$$

We then have $P(\theta) \in R$ for each θ . In addition, each point $P(\theta), \theta \in \mathbb{R}$, is a critical point of the restriction $h|_R$ of the unperturbed Hamiltonian h to the affine space R . It follows that the curve $P(\theta)$ has to be constant if the unperturbed Hamiltonian satisfies the following hypothesis.

Nekhoroshev Steepness

We say that the unperturbed Hamiltonian h is steep if, for each affine subspace Λ in \mathbb{R}^d , the restriction $h|_\Lambda$ has only isolated critical points.

This formulation, due to Niederman, is much simpler than the equivalent one first given by Nekhoroshev. It turns out that this condition, which was made natural by our heuristic explanation, implies stability over exponential timescales for all initial conditions (see Nekhoroshev (1977)). We first need another condition.

Kolmogorov Nondegeneracy

We say that the unperturbed Hamiltonian h is nondegenerate in the sense of Kolmogorov if it has nondegenerate Hessian at each point, or equivalently if the frequency map $p \mapsto \omega(p)$ is an immersion.

Nekhoroshev Stability Theorem

Assume that the unperturbed Hamiltonian does not have critical points ($\omega(p)$ does not vanish), satisfies Nekhoroshev steepness and Kolmogorov nondegeneracy conditions. Then there exists constants $a > 0$ and $b > 0$, which depend only on h , and constants $\epsilon_0 > 0$ and $C > 0$ such that the following holds: for $\epsilon < \epsilon_0$, each trajectory $(q_\epsilon(t), p_\epsilon(t))$ satisfies the estimate

$$\|p_\epsilon(t) - p_\epsilon(0)\| \leq C\epsilon^b$$

for all t such that $|t| \leq e^{C\epsilon^{-a}}$.

Herman's Example

In order to illustrate the necessity of the condition of steepness, let us consider the Hamiltonian

$$H_\epsilon(q_1, q_2, p_1, p_2) = p_1 p_2 + \epsilon V(q_1)$$

with $V: \mathbb{T} \rightarrow \mathbb{R}$. The associated equations are

$$\dot{p}_2 = 0, \quad \dot{p}_1 = -V', \quad \dot{q}_1 = p_2, \quad \dot{q}_2 = p_1$$

The trajectories whose initial conditions are subjected to $p_2(0) = 0$ and $V'(q_1(0)) \neq 0$ satisfy

$$\begin{aligned} p_1(t) &= p_1(0) - t\epsilon V'(q_1(0)) \\ p_2(t) &= 0, \quad q_1(t) = q_1(0) \end{aligned}$$

We see an evolution at speed ϵ of the action variable p_1 contradicting the conclusion of Nekhoroshev theorem. In this example, we have $R(\omega(p(t))) = \mathbb{R} \times \{0\}$, and $h|_{\mathbb{R} \times \{0\}} \equiv 0$, so that the curve

$$P(\theta) = (\theta, 0)$$

is indeed a curve of critical points of $h|_{\mathbb{R} \times \{0\}}$.

Genericity of Steepness

The condition of steepness is frequently satisfied. In order to be more precise, we mention that, for $N \in \mathbb{N}$ large enough (how large depends on the dimension d), steepness is a generic condition in the finite-dimensional space of polynomials of degree less than N . Note in contrast that a quadratic Hamiltonian is steep if and only if it is positive definite. Finally, it is important to mention that convex Hamiltonians h with positive-definite Hessian are steep. More generally, quasiconvex Hamiltonians are steep. A function $h: U \rightarrow \mathbb{R}$ is said to be quasiconvex if, at each point, the restriction of its Hessian to the kernel of its differential is positive definite.

The Quasiconvex Case

It is interesting to be more precise about the values of a and b in Nekhoroshev theorem. We shall do so in the quasiconvex case, which is the most stable case, and where much more is known. If h is quasiconvex, one can take

$$a = b = \frac{1}{2d}$$

as was proved by Lochak (1992). It is a question of active present research whether these exponents are optimal. It now appears that this is almost so, and that the optimal exponent a should not be larger

than $1/2(d-3)$. That this exponent deteriorates as the dimension increases is of course very natural in the perspective of statistical mechanics. As a matter of fact, not only the exponent a but also the threshold ϵ_0 of validity of Nekhoroshev theorem deteriorates with the dimension, as was noticed in Bourgain and Kaloshin.

Another important fact was proved in Lochak (1992): in these expressions, the important value of d is not the total number of degrees of freedom, but the number of active degrees of freedom. More precisely, resonant initial conditions are more stable than generic ones. If r is the order of resonance of a given initial condition, then the number $d-r$ of fast angles can be substituted to the total number of degrees of freedom for the computation of the stability exponent. This phenomenon may account for the surprising stability obtained numerically by Fermi, Pasta, and Ulam.

Permanent Stability

Many initial conditions satisfy more than exponential stability: they are permanently stable.

Kolmogorov Theorem

Assume that h satisfies Kolmogorov nondegeneracy condition ("Kolmogorov nondegeneracy"). Then for each open subset $V \subset \mathbb{R}^d$ such that $\bar{V} \subset U$, there exists $\epsilon_0 > 0$ such that, for each $\epsilon < \epsilon_0$, there exists

- a smooth symplectic embedding $\phi_\epsilon: \mathbb{T}^d \times V \rightarrow \mathbb{T}^d \times U$, which is ϵ -close to the identity,
- a compact subset F_ϵ of V , whose relative measure in V is converging to 1 as $\epsilon \rightarrow 0$,

such that the Hamiltonian system $H_\epsilon \circ \phi_\epsilon$ preserves the torus $\mathbb{T}^d \times \{p\}$ for each $p \in F_\epsilon$.

The union

$$\mathcal{F}_\epsilon = \phi_\epsilon(\mathbb{T}^d \times F_\epsilon)$$

of all the invariant tori has positive measure. Its complement is usually an open dense subset of $\mathbb{T}^d \times U$. All the orbits starting in this invariant set obviously undergo oscillations of amplitude of the order of ϵ for all times. It is worth mentioning that some energy surfaces may not intersect the invariant set \mathcal{F}_ϵ . This is illustrated in example, i.e., "Herman's example," where the surface of zero energy does not contain invariant tori. The following condition guarantees the existence of invariant tori on each energy surface.

Arnol'd Nondegeneracy

The Hamiltonian h is said to be nondegenerate in the sense of Arnol'd if it does not have critical points and if the map

$$p \mapsto \frac{\omega(p)}{\|\omega(p)\|}$$

is a local diffeomorphism between each level set of h and S^{d-1} . This is equivalent to say that the function $(\lambda, p) \in \mathbb{R} \times U \mapsto \lambda h(p)$ has nondegenerate Hessian at each point of the form $(1, p)$.

Arnol'd Theorem

If h satisfies Arnol'd nondegeneracy condition, then the relative measure of the set \mathcal{F}_ϵ of invariant tori is converging to 1 in each energy surface.

This theorem prevents ergodicity of the perturbed systems for the canonical invariant measure on its energy surface. This may be considered as a very disappointing result for statistical mechanics, whose mathematical foundation has often been considered to be the Boltzmann hypothesis of ergodicity. However, statistical mechanics is first of all a question of letting d go to infinity, and ergodicity might not be such a crucial hypothesis (see Khinchin).

When $d=2$, the Arnol'd theorem has particularly strong consequences. Indeed, in this case, the invariant tori cut the energy surfaces in small connected components. The motion is then confined in these connected components. As a consequence, we obtain permanent stability for all initial conditions.

In higher dimensions however, the complement of \mathcal{F}_ϵ in each energy shell is usually a dense, connected open set. There may exist orbits wandering in this large connected set, although the speed of evolution of these orbits is limited by Nekhoroshev theory. Understanding the dynamics in this open set is a very important and difficult question. It is the subject of the next section.

Relaxed Assumption

For many applications, such as celestial mechanics, the nondegeneracy conditions of Arnol'd or Kolmogorov are not satisfied, or difficult to check. However, the existence of invariant tori has been proved under much milder assumptions. As a rule, invariant tori exist in the perturbed systems if the frequency map $p \mapsto \omega(p)$ stably contains Diophantine vectors in its image.

The Mechanism of Arnol'd

Understanding instability is the subject of intense present research. General methods of construction of interesting orbits as well as clever classes of examples are being developed. These methods are exploring the limits of stability theory. Here we shall only describe the fundamental ideas of Arnol'd (see Arnol'd 1964), where most of the present activity finds its roots. Although these ideas have some ambition of universality, they are best presented, like in Arnol'd (1964), on an example. We consider the quasiconvex Hamiltonian

$$\begin{aligned} H(q_1, q_2, q_3, p_1, p_2, p_3) \\ = (p_1^2 + p_2^2)/2 - p_3 + \epsilon \cos 2\pi q_2 \\ + \mu(\cos 2\pi q_2)(\cos 2\pi q_1 + \cos 2\pi q_3) \end{aligned}$$

As we have seen, this system is typical of the kind of Hamiltonians one gets after reduction to resonant normal form. However, it is illuminating to consider μ not as a function of ϵ but as an independent parameter. This is an idea of Poincaré then followed by Arnol'd. We shall expose the main steps of the proof of the following result.

Theorem

Let us fix numbers $0 < A < B$. For each $\epsilon > 0$, there exists a number $\mu_0(\epsilon)$ such that, when $0 < \mu < \mu_0(\epsilon)$, there exists a trajectory

$$(q_1(t), q_2(t), p_1(t), p_2(t))$$

and a time $T > 0$ (which depends on ϵ and μ) such that

$$p_1(0) \leq A, \quad p_1(T) \geq B$$

The Truncated System

Let us begin with some remarks about the truncated Hamiltonian obtained when $\mu=0$:

$$\begin{aligned} H_0(q, p) &= H_1(q_1, q_3, p_1, p_3) + H_2(q_2, p_2) \\ &= p_1^2/2 - p_3 + p_2^2/2 + \epsilon \cos 2\pi q_2 \end{aligned}$$

This system is the uncoupled product of H_1 and of the pendulum described by H_2 . The variable p_1 is constant along motion; hence, the theorem can not hold for $\mu=0$.

Recall that the point $q_2=0, p_2=0$ is a hyperbolic fixed point of the pendulum $H_2(q_2, p_2)=p_2^2/2 + \epsilon \cos 2\pi q_2$. The stable and unstable manifolds of this integrable system coincide; they form the energy level $H_2=\epsilon$. As a consequence, in the product system of Hamiltonian $H_0=H_1+H_2$, there exists,

in the zero energy level, a one-parameter family T_ω of invariant tori of dimension 2:

$$T_\omega = \{p_1 = \omega, p_3 = \omega^2/2 + \epsilon, q_2 = 0, p_2 = 0\} \\ \subset \mathbb{T}^3 \times \mathbb{R}^3$$

Each of these tori is hyperbolic in the sense that it has a stable manifold of dimension 3 and an unstable manifold of dimension 3, which are nothing but the liftings of the stable and unstable manifolds of the hyperbolic fixed point of H_2 . Notice that these manifolds do not intersect transversally along T_ω .

When $\mu \neq 0$, the perturbation is chosen in such a way that the tori T_ω are left invariant by the Hamiltonian flow.

Splitting

For $0 < \mu < \mu_0(\epsilon)$, the invariant tori T_ω still have stable and unstable manifolds of dimension 3. These stable and unstable manifolds intersect transversally in the energy surface, along an orbit which is homoclinic to the torus.

The first point is that the tori remain hyperbolic, and that the stable and unstable manifolds are deformed, but not destroyed by the additional term. This results from the observation that the manifold M formed by the union of the invariant tori is normally hyperbolic in its energy surface. Note that this step does not require exponential smallness of μ .

It is then a very general result that the stable and unstable manifolds have nonempty intersection. It is a global property, which can be established by variational methods, and which still does not rest on exponential smallness of μ .

The key point, where exponential smallness is required, is transversality. Since transversality is a generic phenomenon, one may think that this step is not so crucial. And indeed, it is very likely that the statement remains true for most values of $\mu \in]0, \epsilon]$ (and not only for $\mu \leq \mu_0(\epsilon)$). However, there are two important issues here. First, transversality is difficult to establish on explicit examples. Second, it is useful for many further discussions to obtain some quantitative estimates.

Indeed, we can associate to the intersection between the stable and unstable manifolds a quantity, the splitting, which in a sense measures transversality. Discussions on such a definition are available in Lochak *et al.* (2003). Using methods of Poincaré and Melnikov, Arnol'd showed that this splitting can be estimated, for sufficiently small ϵ , by

$$\alpha \geq \mu e^{-C/\sqrt{\epsilon}} + O(\mu^2) \quad [3]$$

This implies non-nullity of the splitting, hence transversality, for small μ .

Transition Chain

We have established the existence, when $\mu > 0$ is small enough, of a family T_ω of hyperbolic invariant tori such that the stable manifold W_ω^+ and the unstable manifold W_ω^- intersect transversally along a homoclinic orbit (but not along T_ω !) for each ω .

A stability argument shows that the stable manifold W_ω^+ of the torus T_ω intersects transversally the stable manifold $W_{\omega_0}^-$ of the torus T_{ω_0} when ω is close enough to ω_0 . How close directly depends on the size of the splitting. We obtain heteroclinic orbits between tori close to each other.

Given two values ω and ω' , we can find a sequence $\omega_i, 1 \leq i \leq N$, such that $\omega_0 = \omega, \omega_N = \omega'$, and W_i^- intersects transversally W_{i+1}^+ for all i . The associated family T_{ω_i} of tori is called a transition chain.

The left step consists in proving that some orbits shadow the transition chain. Arnol'd solved this step by a very simple topological argument which, however, does not provide any estimate on the time T . He proves the existence of an orbit joining any neighborhood of T_ω to any neighborhood of $T_{\omega'}$. This ends the proof of the main theorem, since we can choose ω and ω' such that $\omega < A < B < \omega'$.

The dynamics associated to hyperbolic tori and transition chains have later been studied more carefully. In particular, a λ -lemma can be proved in this context, which allows us to conclude that, in a transition chain, the unstable manifold W_0^- of the first torus intersects transversally the stable manifold of the last torus W_N^+ . These detailed studies also allow us to relate the speed of diffusion to the splitting of the invariant manifolds.

Diffusion Speed

It is interesting to estimate the speed of evolution of the variable p_1 , or in other words the time T in the statement. It follows from Nekhoroshev theory that this time T has to be exponentially large as a function of ϵ . In fact, it is possible to prove, either by recent developments on the ideas of Arnol'd exposed above, or more easily by variational methods, (Bessi 1996) that

$$T \leq \frac{e^{C/\sqrt{\epsilon}}}{-\mu \log \mu}$$

for $\mu \leq \mu_0(\epsilon)$. This time is of course highly related to the estimate [3] of the splitting. In addition, Ugo Bessi proved that one can take $\mu_0(\epsilon) = e^{-C/\sqrt{\epsilon}}$. Plugging this value of μ in the estimate of T , we get the estimate $T \leq e^{C/\sqrt{\epsilon}}$ as a function of the only parameter ϵ .

Considering the fact that the orbit we have described goes close to double resonances, this is the best estimate one may hope for in view of the improved Nekhoroshev stability estimates at resonances.

The idea is now well spread that the time of diffusion is exponentially large. However, we point out that, if it is indeed exponentially small as a function of the parameter ϵ , it is only polynomially small as a function of the second parameter μ , as was first understood by P Lochak and proved in Bernard (1996) using the variational method of U Bessi.

Conclusion

The theories of instability are developing in several directions. One of them is to try to understand the limits of stability, and to test to what extent the stability results obtained so far are optimal. This aspect has quickly developed recently, for example, the optimal stability exponent a for convex systems is almost known. Another direction is to try to give a description of unstable orbits in typical systems. This remains a widely open question.

Let us finally mention that the application of the theories we have presented to concrete systems is very difficult. One of the reasons is that the estimates of the threshold ϵ_0 of validity of Nekhoroshev and KAM theorems that can (painfully) be obtained by inspection in the proofs are very bad, and it is much too bad, for example, to think about applications to the solar systems with the physical values of the parameters.

See also: Averaging Methods; Hyperbolic Billiards; KAM Theory and Celestial Mechanics; Separatrix Splitting; Stability Problems in Celestial Mechanics; Stability Theory and KAM; Weakly Coupled Oscillators.

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Hamilton–Jacobi Equations and Dynamical Systems: Variational Aspects

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Overview

Given a continuous Hamiltonian $H(x, p)$ defined on the cotangent bundle of a compact boundaryless manifold, where x and p are the state and the momentum variable, respectively, and satisfying suitable convexity and coercivity assumptions, we consider the family of Hamilton–Jacobi equations

$$H(x, D\phi) = a \quad [1]$$

with a a real parameter. If, in addition, H is assumed to be smooth, we also consider the Hamilton's equations

$$\dot{\xi} = H_p(\xi, \eta), \quad \dot{\eta} = -H_x(\xi, \eta) \quad [2]$$

whose analysis is related to the variational problem of minimizing the action functional

$$\int_I L(\xi, \dot{\xi}) dt \quad [3]$$

among all Lipschitz-continuous or, equivalently, continuous piecewise C^1 curves defined on I with fixed end points. Here I is a compact interval and L , the Lagrangian, is the Fenchel transform of H . A “conjugate” flow, named after Euler–Lagrange, is

also defined on the tangent bundle of the underlying manifold.

A connection between [1] and [2] is provided by the classical Hamilton–Jacobi method, which shows that the graph of the differential of any regular, say C^1 , global solution to [1] is an invariant subset for the Hamiltonian flow. The drawback of this approach is that such regular solutions do not exist in general, even for very regular Hamiltonians.

However, for any continuous Hamiltonian a distinguished value of the parameter a can be detected, denoted by c and qualified, from now on, as critical, for which there are a.e. subsolutions of the corresponding Hamilton–Jacobi equations enjoying some extremality properties. Note that such functions can be equivalently defined as weak solutions, in the viscosity sense, of [1] with $a=c$, or as fixed points of the associated Lax–Oleinik semigroup (see Fathi (to appear)). We do not give these interpretations here to avoid any technicalities.

Even if they are just Lipschitz–continuous on the whole underlying manifold, these extremal subsolutions become of class C^1 , when restricted on a special compact subset, the same for any of them, say \mathcal{A} , and the corresponding differentials coincide on \mathcal{A} . More generally, all critical subsolutions, that is, the a.e. subsolutions to [1] with $a=c$, are continuously differentiable on \mathcal{A} . This regularity property holds if H is at least locally Lipschitz–continuous in both variables. When, in addition, the Hamiltonian is smooth, so that the Hamiltonian flow is defined, the graph of this common differential defined in \mathcal{A} , denoted by $\tilde{\mathcal{A}}$, is an invariant set for the flow, and is foliated by integral curves of [1] possessing some global minimizing properties with respect to the action functional.

The aim of this presentation is to give an explanation of the previously described phenomena occurring at the critical level, and of some related facts, using tools and arguments as simply as possible. We propose a metric approach to the subject and consider as central in our analysis a family of distances, denoted by S_a , for any $a \geq c$. We emphasize that such distances can be defined for only continuous Hamiltonians, and the qualitative analysis of the critical subsolutions has an interest independent from the dynamical applications. Indeed, it can be used in other contexts such as in homogenization problems, and the large-time behavior of the viscosity solutions to the time-dependent equation $u_t + H(x, Du) = 0$.

The discovery of the critical value has a history that reflects the dual character of the topics, which has a dynamical as well as a partial differential equation (PDE) interest.

It was probably Ricardo Mañé who first focused his attention on it, at the beginning of the 1980s, in connection with the analysis of integral curves of the Euler–Lagrange flow with some global minimizing properties. The set, previously denoted by $\tilde{\mathcal{A}}$, has been found and analyzed by Serge Aubry, in a purely dynamical way, as the union of the supports of such minimizing curves. On the other hand, John Mather (1986) independently defined, in a more general framework, a set, contained in the Aubry set, through a weak approach that utilizes minimal probability measures invariant with respect to the Euler–Lagrange flow. The Mather set is actually the closure of the union of the supports of such measures. We will follow the approach of Aubry (see Fathi (2005b)), and will not introduce the Mather’s measures.

In the viscosity solution theory, the critical value has instead been introduced in a famous unpublished paper of P L Lions, S R S Varadhan, and G Papanicolaou (1987), in connection with some periodic homogenization problems for Hamilton–Jacobi equations. It is worth noticing that they consider continuous Hamiltonian, defined on the flat N -dimensional torus, without any convexity assumption.

They define the critical value, and show the existence of viscosity solutions to the critical equation by means of an ergodic approximation, that is, by considering the equation $\varepsilon u + H(x, Du) = 0$ and then passing to the limit for $\varepsilon \rightarrow 0$. The critical viscosity solutions are used as correctors in the homogenization. They do not perform any qualitative analysis, and if such analysis can be done, and something similar to the Aubry–Mather sets exists for nonconvex Hamiltonian this is still an important open problem.

The two pieces of the picture were pasted together by Fathi (1996) with his weak KAM theory (see Contreras and Iturriaga (1999) and Fathi (2005a) for a general treatment, where the relevance of the extremal critical subsolutions has first been recognized for the analysis of the dynamics, and the Aubry–Mather sets have been characterized as a regularity set for such subsolutions, as described above). Evans and co-workers have been presently using more general PDE methods in weak KAM theory to address some integrability issues and to find a quantum analog (see Evans and Gomes (2001, 2002) and Evans (2004)).

Critical Value and Extremal Subsolutions

We consider the family of Hamilton–Jacobi equations [1] defined, for simplicity, on the flat torus $T^N = \mathbb{R}^N / \mathbb{Z}^N$, endowed with the flat Riemannian

metric induced by the Euclidean metric on \mathbb{R}^N . The tangent, as well as the cotangent bundle of \mathbb{T}^N will be identified with $\mathbb{T}^N \times \mathbb{R}^N$. All the results discussed in the remainder of the paper are still true in any compact boundaryless manifold, and some of them also hold in noncompact manifolds. We require H to be continuous in both variables, to satisfy the coercivity assumption,

$\{(y, p): H(y, p) \leq a\}$ is compact for any a

and the following (strict) quasiconvexity conditions for any $x \in \mathbb{T}^N$, $a \in \mathbb{R}$:

$\{p: H(x, p) \leq a\}$ is strictly convex
 $\partial\{p: H(x, p) \leq a\} = \{p: H(x, p) = a\}$

where ∂ , in the above formula, indicates the boundary. We denote by \mathcal{S}_a the (possibly empty) set of the Lipschitz-continuous a.e. subsolutions to [1]. They will be called in the sequel, for short, just subsolutions. Due to the convex character of the Hamiltonian and its continuity, the property of being a subsolution, for some function u , can be equivalently expressed by requiring the inequality $H(x, p) \leq a$ to hold for any $x \in \mathbb{T}^N$ and any p in the (Clarke) generalized gradient $\partial u(x)$, defined by

$$\partial u(x) = \text{co}\{p = \lim_i Du(x_i): \\ x_i \text{ differentiability point of } u, \lim_i x_i = x\}$$

where co indicates the convex hull. Note that if this set of weak derivatives reduces to a singleton at some x , then the function u is strictly differentiable at x , i.e., it is differentiable and Du is continuous at x .

By a strict subsolution to [1] we mean a Lipschitz-continuous function w with $\text{ess sup}_{\mathbb{T}^N} H(x, Dw(x)) < a$. The property of being a (strict) subsolution is not affected by addition of constants. Moreover, the pointwise supremum (resp. infimum) of any class of equibounded subsolution to [1] is itself a subsolution, and \mathcal{S}_a is stable with respect to the uniform convergence in \mathbb{T}^N .

The purpose of this section is to show that there is a unique value c (the critical value) for which the corresponding equation

$$H(x, Du) = c \quad [4]$$

possesses subsolutions enjoying some extremality properties. We, more precisely, call a subsolution $u \in \mathcal{S}_a$ maximal (resp. minimal) if for any open subset Ω of \mathbb{T}^N and any Lipschitz-continuous function ϕ with $u = \phi$ on $\partial\Omega$ and $\text{ess sup}_{\Omega} H(x, D\phi(x)) < a$ [5] one has $u \geq \phi$ (resp. $u \leq \phi$) in Ω .

Any maximal (resp. minimal) subsolution u is actually an a.e. solution of [1]. If, in fact, $H(x_0, Du(x_0)) < a$ for some differentiability point x_0 of u , then the function $\phi(x) = u(x_0) + Du(x_0)(x - x_0) - \varepsilon|x - x_0| + \varepsilon$ (resp. $\phi(x) = u(x_0) + Du(x_0)(x - x_0) + \varepsilon|x - x_0| - \varepsilon$) should satisfy [5] for a suitable choice of $\varepsilon > 0$ and of a neighborhood Ω of x_0 , and so should violate the maximality (resp. minimality) condition for u .

The previous argument can be easily adapted to show something more general: if u is a maximal (resp. minimal) subsolution then no subtangents (resp. supertangents) to u at any $y \in \mathbb{T}^N$ can be local strict subsolutions at y , that is, strict subsolutions in some neighborhood of y .

The subtangency (resp. supertangency) condition of a function ϕ to u at a point x_0 means that x_0 is a local minimizer (resp. maximizer) of $u - \phi$. We denote by $D^-u(x_0)$ (resp. $D^+u(x_0)$) the sets made up by the differentials of the C^1 -subtangent (resp. supertangent) to u at x_0 . They are (possibly empty) closed convex subsets of $\partial u(x_0)$. It is apparent that if $D^+u(x_0) \neq \emptyset \neq D^-u(x_0)$ then u is differentiable at x_0 and $D^+u(x_0) = D^-u(x_0) = \{Du(x_0)\}$.

It is an immediate consequence of the previous fact that no extremal subsolutions can exist in \mathcal{S}_a , whenever [1] admits a strict subsolution, say ϕ , since there are global minimizers and maximizers of $u - \phi$, for any $u \in \mathcal{S}_a$, because of the compactness of \mathbb{T}^N . The function ϕ is then subtangent and supertangent, respectively, to u at such points.

The unique value we can look at for finding extremal subsolutions is therefore

$$c = \inf\{a \in \mathbb{R}: \mathcal{S}_a \neq \emptyset\} \quad [6]$$

The set on the right-hand side of [6] is nonempty since the null function belongs to \mathcal{S}_a when $a > \max_{\mathbb{T}^N} H(x, 0)$, and bounded from below by $\min_{\mathbb{T}^N} H(x, 0)$. The value c is consequently well defined by [6].

Moreover, any sequence $u_n \in \mathcal{S}_{a_n}$, with a_n decreasing and convergent to c , is equi-Lipschitz-continuous because of the coercivity of H , and equibounded, up to addition of suitable constants. It is therefore uniformly convergent, up to a subsequence, to some u , which belongs to \mathcal{S}_{a_n} , for any n , since these classes are stable for the uniform convergence. This implies that u is a subsolution to [4], so that $\mathcal{S}_c \neq \emptyset$. The critical value c is then characterized by the property that the corresponding eqn [4] admits subsolutions but not strict subsolutions. Our aim is to show that extremal subsolutions do exist for the critical eqn [4].

For any supercritical value a , that is, $a \geq c$, we can define the functional nonsymmetric semidistance:

$$\begin{aligned} S_a(y, x) &= \sup\{u(x) - u(y) : u \in \mathcal{S}_a\} \\ &= \sup\{u(x) : u \in \mathcal{S}_a, u(y) = 0\} \end{aligned}$$

for any x, y in \mathbb{T}^N . It is immediate that S_a satisfies the triangle inequality and $S_a(y, y) = 0$ for any y . But it fails, in general, to be symmetric and positive if $x \neq y$. We will nevertheless call it a distance, in the sequel, to ease terminology. The function $x \mapsto S_a(y, x)$ is itself a subsolution to [1], for any y , being the pointwise supremum of a family of equibounded subsolutions. Taking into account the inequality

$$u(x) - u(y) \geq -S_a(x, y)$$

which holds for any $u \in \mathcal{S}_a$, and the fact that it becomes an equality by setting $u = S_a(x, \cdot)$, we also get

$$\begin{aligned} -S_a(x, y) &= \inf\{u(x) - u(y) : u \in \mathcal{S}_a\} \\ &= \inf\{u(x) : u \in \mathcal{S}_a, u(y) = 0\} \end{aligned}$$

and $-S_a(\cdot, y)$ is, as well, a subsolution to [1]. Note that

$$S_a(x, y) + S_a(y, x) \geq 0 \quad \text{for any } y, x \quad [7]$$

The interest of introducing the distance S_a in the present context is that, for any $a \geq c$ and $y \in \mathbb{T}^N$, the function $x \mapsto S_a(y, x)$ (resp. $x \mapsto -S_a(x, y)$) satisfies the maximality (resp. minimality) condition for subsolutions of [1] in any open set not containing y . If, by contradiction, the maximality property of $S_a(y, \cdot)$ were violated in some open set Ω with $y \notin \Omega$ by a ϕ satisfying [5] then one could make the set $\{x : \phi(x) > S_a(y, x)\}$ nonempty and compactly contained in Ω , by adding a suitable constant. Hence, the formula

$$u = \begin{cases} \max\{\phi, S_a(y, \cdot)\} & \text{in } \Omega \\ S_a(y, \cdot) & \text{otherwise} \end{cases} \quad [8]$$

could provide a subsolution to [1] with $u(y) = S_a(y, y) = 0$ and $u > S_a(y, \cdot)$ at some point of Ω , which is in contrast with the very definition of S_a . One can similarly prove the minimality condition for $-S_a(\cdot, y)$.

We now focus our attention on the critical case. We derive from the previous considerations that if a maximal subsolution to [4] does not exist then, for any y , we can find a neighborhood Ω_y of y where $S_c(y, \cdot)$ fails to be maximal. We can thus construct, through a formula like [8], a $u_y \in \mathcal{S}_c$ with

$$\text{ess sup}_{\Omega_y} H(\cdot, Du_y(\cdot)) < c \quad [9]$$

in some neighborhood Ω_y of y contained in Ω'_y . Thanks to the compactness of \mathbb{T}^N , we can extract from $\{\Omega_y\}$ a finite subcover $\{\Omega_{y_i}\}, i = 1, \dots, m$, for some $m \in \mathbb{N}$, and define

$$u = \sum_i \lambda_i u_{y_i}$$

where λ_i are positive constants with $\sum_1^m \lambda_i = 1$. The convex character of the Hamiltonian and [9] imply that u is a strict critical subsolution, which cannot be. We therefore conclude that there is a nonempty subset of y , denoted henceforth by \mathcal{A} , for which $S_c(y, \cdot)$ is indeed a maximal critical subsolution. It can also be proved, by exploiting some stability properties of the maximal subsolutions, that \mathcal{A} is closed. Similarly, $-S_a(\cdot, y)$ must be a minimal critical subsolution for some y . We denote by $\bar{\mathcal{A}}$ the closed set made up by such points.

The previous covering argument shows that if $y \notin \mathcal{A}$ (resp. $y \notin \bar{\mathcal{A}}$) then there is a local strict critical subsolution at y . The converse is also true: let in fact ϕ be such a strict subsolution satisfying $\phi(y) = S_c(y, y) = 0$; then ϕ is sub-tangent to $S_c(y, \cdot)$ (resp. super-tangent to $-S_c(\cdot, y)$) at y , by the very definition of the distance S_c . This shows that $S_c(y, \cdot)$ (resp. $-S_c(\cdot, y)$) is not a maximal (resp. minimal) critical subsolution, and so $y \notin \mathcal{A}$ (resp. $y \notin \bar{\mathcal{A}}$). Since the previous characterization holds for both \mathcal{A} and $\bar{\mathcal{A}}$, it follows that $\mathcal{A} = \bar{\mathcal{A}}$. This set is a generalization of the (projected) Aubry set. We will come back on this point later on.

We also see from the covering argument that there is a critical subsolution ϕ , which is strict outside \mathcal{A} , that is, such that $\text{ess sup}_{\Omega} H(x, D\phi(x)) < c$ for any open set Ω compactly contained in $\mathbb{T}^N \setminus \mathcal{A}$.

This implies that any y such that $\{p : H(y, p) \leq c\}$ has empty interior, belongs to \mathcal{A} . The empty interior condition in fact implies, thanks to the strict quasiconvexity of H , that the sublevel set reduces to a singleton, say $\{p_0\}$. We know that $\partial u(y) \subset \{p : H(y, p) \leq c\}$, for any $u \in \mathcal{S}_c$; therefore, $\partial u(y)$ is a singleton and so any critical subsolution u is strictly differentiable at y with $H(y, Du(y)) = H(y, p_0) = c$. Hence, there cannot be critical subsolutions which are strict around y .

The previously described points will be called, in the sequel, equilibria, and the (possibly empty) closed set made up by them will be denoted by \mathcal{E} . The reason of this terminology will be explained later. The differentiability property of the critical subsolutions at equilibria, can be extended, quite surprisingly, to any point of \mathcal{A} , under more stringent assumptions on H . We will discuss this issue in the next section.

Qualitative Properties of Generalized Aubry Set

We introduce some dynamical aspects in the picture by showing that the distances S_a , defined in the previous section for any $a \geq c$, are actually of length type, in the sense that $S_a(y, x)$ equals, for any pair y, x , the infimum of the intrinsic length of absolutely continuous, or equivalently Lipschitz-continuous, curves joining y to x . By intrinsic length, we mean the total variation of S_a on the curve. It will be denoted by ℓ_a , while ℓ will indicate the natural (i.e., Euclidean) length.

For this purpose, we proceed to give a line-integral representation formula of S_a . To start with, we consider a C^1 subsolution u to [1], some $x, y \in \mathbb{T}^N$ and a (Lipschitz-continuous) curve ξ , defined in some compact interval I , joining y to x . We have

$$u(x) - u(y) = \int_I Du \dot{\xi} dt \leq \int_I \sigma_a(\xi, \dot{\xi}) dt \quad [10]$$

where, for any $(x, v) \in \mathbb{T}^N \times \mathbb{R}^N$, $\sigma_a(x, v) := \max_{p \in Z_a(x)} p \cdot v$ and

$$Z_a(x) := \{p: H(x, p) \leq a\}$$

Inequality [10] also holds for a Lipschitz-continuous subsolution to [1] through suitable replacement of the differential by the generalized gradient. The set-valued map Z_a is compact convex valued, by the coercivity and quasiconvexity assumptions on H , and continuous with respect to the Hausdorff metric. The function σ_a is accordingly continuous in the first variable, and convex and positively homogeneous in the second, being a support function. This implies in particular that the integral on the right-hand side of [10] is invariant under change of parameter preserving the orientation. We derive, from [10],

$$S_a(y, x) \leq \inf \left\{ \int_0^1 \sigma_a(\xi, \dot{\xi}) dt: \xi \text{ defined in } [0, 1] \text{ and joining } y \text{ to } x \right\} \quad [11]$$

for any y, x . We denote by $\bar{S}_a(y, x)$ the quantity on the right-hand side of [11]. It is immediate that the triangle inequality holds for \bar{S}_a . The function $u := \bar{S}_a(y, \cdot)$ is, moreover, Lipschitz-continuous since $\sigma_a(x, v)/|v|$ is bounded from above in $\mathbb{T}^N \times (\mathbb{R}^N \setminus \{0\})$ because of the coercivity of H . Given $v \in \mathbb{R}^N$, we exploit the definition of \bar{S}_a , the continuity of σ_a , and the triangle inequality for \bar{S}_a , to get at any differentiability point x_0 of u ,

$$\begin{aligned} Du(x_0)v &= \lim_{h \rightarrow 0^+} \frac{u(x_0 - hv) - u(x_0)}{h} \\ &\leq \limsup_{h \rightarrow 0^+} \frac{\bar{S}_a(x_0 - hv, x_0)}{h} \\ &\leq \lim_{h \rightarrow 0^+} \frac{1}{h} \int_0^1 \sigma_a(x_0 - hvt, hv) dt \\ &= \lim_{h \rightarrow 0^+} \int_0^1 \sigma_a(x_0 - hvt, v) dt \\ &= \sigma_a(x_0, v) \end{aligned}$$

This implies by Hahn–Banach theorem that $Du(x_0) \in Z_a(x_0)$ or, in other terms, that $u = \bar{S}_a(y, \cdot) \in S_a$. We then derive, from [11] and the very definition of S_a ,

$$S_a(y, x) = \inf \left\{ \int_0^1 \sigma(\xi, \dot{\xi}) dt: \begin{array}{l} \xi \text{ defined in } [0, 1] \text{ with } \xi(0) = y, \\ \xi(1) = x \end{array} \right\}$$

Taking into account that the integral functional appearing in the previous formula is lower semicontinuous for the uniform convergence of equi-Lipschitz-continuous sequence of curves, by standard variational results, we in turn infer that it equals the intrinsic length ℓ_a . Mathematically,

$$\ell_a(\xi) = \int_I \sigma_a(\xi, \dot{\xi}) dt$$

for any compact interval I and any curve ξ defined in I .

Since S_a is just a semidistance, we do not have any *a priori* information on the sign of ℓ_a ; however, by [10], the intrinsic length of any cycle must be non-negative. Furthermore, while $|\ell_a(\xi)|$ must be small for any curve ξ with small natural length, by the coercivity condition on H , no converse estimates hold, in general. If $a > c$, some information in this direction can be gathered by taking a strict subsolution ϕ to [1], that it can be assumed smooth, up to regularization by mollification, then $D\phi(x)v \leq \sigma_a(x, v) - \rho|v|$ for any $(x, v) \in \mathbb{T}^N \times \mathbb{R}^N$, and some $\rho > 0$, and consequently

$$\begin{aligned} \ell_a(\xi) &\geq \int_I (\sigma_a(\xi, \dot{\xi}) - D\phi(\xi)\dot{\xi}) dt \\ &+ \phi(x) - \phi(y) \geq \rho \ell(\xi) - S_a(x, y) \quad [12] \end{aligned}$$

for any pair y, x and any curve ξ , defined in some interval I , joining y to x . The previous formula says, in particular, that when $|x - y|$ is small then any curve whose intrinsic length approximates $S_a(y, x)$ must have small natural length. The previous

argument cannot be extended to the critical case. This gap suggests the next definition. The main purpose for introducing it is to get a metric characterization of the Aubry set \mathcal{A} .

We say that S_c is localizable at some y if for every $\varepsilon > 0$ there is $0 < \delta_\varepsilon < \varepsilon$ such that

$$S_c(y, x) = \inf\{\ell_c(\xi) : \xi \text{ joins } y \text{ to } x \text{ and } \ell(\xi) < \varepsilon\} \quad [13]$$

whenever $|x - y| < \delta_\varepsilon$. If $y \notin \mathcal{A}$, we adapt the argument previously used in the strict subcritical case to get that S_c is indeed localizable at y . In this case we have, in fact, at our disposal a critical subsolution, say ϕ , which is strict in some neighborhood Ω of y , thanks to the characterization of the Aubry set given in the previous section.

We assume, to simplify, ϕ to be C^1 ; under the natural condition of Lipschitz-continuity, generalized gradients should be used in place of differentials. We have $D\phi(x)v \leq \sigma(x, v) - \rho|v|$ for any $x \in \Omega$, any $v \in \mathbb{R}^N$, and some $\rho > 0$, and $D\phi(x)v \leq \sigma(x, v)$, for any x, v . Exploiting these inequalities, we obtain an estimate analogous to [12] for curves starting from y , which allows us to prove [13].

Conversely, let $y \notin \mathcal{E}$ be a point where S_c is localizable. We claim that $Z_c(y) \subset D^-u(y)$, where $u := S_c(y, \cdot)$. It is enough to show that any p_0 in the interior of $Z_c(y)$ belongs to $D^-u(y)$, since $D^-u(y)$ is closed. Note that the interior of $Z_c(y)$ is nonempty since we are assuming that y is not an equilibrium. Such a p_0 belongs to the interior of $Z_c(x)$ for x sufficiently close to y , thanks to the continuity of Z_c ; consequently, $p(x - y) < \ell_c(\xi)$ for any x close to y and any curve ξ joining y to x with $\ell(\xi)$ sufficiently small. Taking into account [13], we then deduce

$$p(x - y) \leq S_c(y, x) \quad \text{for } x \text{ close to } y$$

and so the linear function $\phi(x) := p_0(x - y)$ is subtangent to u at y . This in turn implies that y is out of \mathcal{A} since ϕ is a local strict critical subsolution at y , and so $S_c(y, \cdot)$ cannot be a maximal subsolution by the characterization given in the previous section.

The fact that S_c is not localizable at any point of $y \in \mathcal{A} \setminus \mathcal{E}$ leads to the announced metric characterization of \mathcal{A} . If y is such a point, there is an $\varepsilon > 0$, a point x , with $|x - y| < \varepsilon$, and so $|S_c(y, x)|$, as small as desired, and a curve ξ joining y to x with $\ell_c(\xi) \sim S_c(y, x)$ and $\ell(\xi) > \varepsilon$. We construct a cycle γ , passing through y , by juxtaposition of ξ and the Euclidean segment joining x to y . We obtain, in this way, a sequence of cycles γ_n , passing through y , with length $\ell_c(\gamma_n) \rightarrow 0$ and $\ell(\gamma_n) \geq \varepsilon$, for any n .

The same result can also be obtained for $y \in \mathcal{E}$. In this case we select $\varepsilon > 0$ and $v_0 \in \mathbb{R}^N$ with $\sigma_c(y, v_0) = 0$, and denote by B_n a sequence of

Euclidean balls, centered at y , satisfying $\sigma_c(\cdot, v_0) < 1/n$ in B_n . We construct a sequence of cycles, passing through y , by going up and down on the line $\{y + sv\}$ in such a way that $\gamma_n(t) \in B_n$, for every t , and $\varepsilon < \ell(\gamma_n) < 2\varepsilon$; therefore $0 \leq \ell_c(\gamma_n) < 2\varepsilon/n$.

Conversely, such a sequence of cycles cannot exist at any $y \notin \mathcal{A}$ because S_c is localizable at y .

We emphasize that the previous definition of \mathcal{A} through cycles and the fact that S_c is not localizable at any point $y \in \mathcal{A}$ with $\text{int}Z_c(y) \neq \emptyset$ shows that, apart for the special case of equilibria, the property of being a point of \mathcal{A} is definitively not of local nature.

As pointed out already, if $y \notin \mathcal{A}$, and so S_c is localizable at y , then $Z_c(y) \subset D^-u(y)$, where $u := S_c(y, \cdot)$; on the other hand, we know that $D^-u(y) \subset \partial u(y)$ and $\partial u(y) \subset Z_c(y)$, where the latter inclusion holds since u is a critical subsolution. We then derive

$$D^-u(y) = \partial u(y) = Z_c(y)$$

We interpret these inequalities as a convexity-type property, or, to use a more appropriate terminology, a semiconvexity property of the distance function $S_c(y, \cdot)$ at y . The same property holds for the Euclidean distance function $|x|$ at 0.

A contrasting phenomenon takes place if $y \in \mathcal{A}$, namely $S_c(y, \cdot)$ is semiconcave at y , which means that $D^+u(y) = \partial u(y)$. This is more complicated to prove (see Fathi 2005b), and requires, in addition, H to be strictly convex in p and locally Lipschitz-continuous in (x, p) . Under these assumptions one can, more generally, show that $S_c(y, \cdot)$ is semiconcave in \mathbb{T}^N , if $y \in \mathcal{A}$, while it is semiconcave in $\mathbb{T}^N \setminus \{y\}$ and semiconvex in y , if $y \notin \mathcal{A}$. Some important consequences can be deduced.

First, thanks to the semiconcavity property there are C^1 supertangents to $u := S_c(y, \cdot)$ at y , whenever $y \in \mathcal{A}$. Such a function, say ϕ , is also supertangent to $-S_c(\cdot, y)$, which is a minimal critical subsolution, at the same point. We know from the previous section that no supertangents to $-S_c(\cdot, y)$ at y can be strict critical subsolution locally at y , and so $H(y, D\phi(y)) = c$. This implies that $D^+u(y)$ is contained in the boundary of $Z_c(y)$. We then see, taking into account that $D^+u(y)$ is convex and $Z_c(y)$ strictly convex, that $D^+u(y)$ reduces to a singleton, and so, by the semiconcavity property, $\partial u(y)$ reduces to a singleton. Therefore, $S_c(y, \cdot)$ is strictly differentiable at y , for any $y \in \mathcal{A}$. One can similarly show that $-S_c(\cdot, y)$ is strictly differentiable at y .

Second, given $y \in \mathcal{A}$ and a critical subsolution w , which can be assumed, up to addition of a constant, to vanish at y , we see that $S_c(y, \cdot)$ (resp. $-S_c(\cdot, y)$) is supertangent (resp. subtangent) at y because of its extremality properties. Since both these

super(sub)-tangents are differentiable, by the previous point, we deduce that w itself is differentiable at y . Moreover, the differentials at y of all three functions under consideration, namely $S_c(y, \cdot)$, $-S_c(\cdot, y)$, and w , coincide. In particular, $H(y, Dw(y)) = c$, and $y \mapsto Dw(y)$ is continuous on \mathcal{A} , since $S_c(y, \cdot)$ has been proved to be strictly differentiable at y , whenever $y \in \mathcal{A}$. Any critical subsolution, restricted to \mathcal{A} , is consequently a continuously differentiable solution to [4].

Summing up, we have discovered (under the assumption of strict convexity and Lipschitz-continuity for H) that every critical subsolution is differentiable on \mathcal{A} , and the differential on \mathcal{A} is the same for every critical subsolution. A continuous map $G: \mathcal{A} \rightarrow \mathbb{R}^N$ is then defined by taking $G(y)$ equal to the common differential of any critical subsolution at y . We denote by $\tilde{\mathcal{A}}$ the graph of G , which is a subset of the cotangent bundle of \mathbb{T}^N , identified with $\mathbb{T}^N \times \mathbb{R}^N$.

As we have already pointed out, the existence of a C^∞ subsolution to [1] is obvious when $a > c$, and such a subsolution can be obtained through a suitable regularization by mollification of any strict subsolution. The same construction cannot be performed at the critical level, since no strict critical subsolutions are available to start the regularization procedure. We can nevertheless show the existence of C^1 critical subsolutions by exploiting the information gathered on the Aubry set. We start by considering a countable locally finite open cover of $\mathbb{T}^N \setminus \mathcal{A}$, $\{\Omega_i\}$; we know from the previous section that there is a critical subsolution, say w_i , which is strict on Ω_i , for any i . Loosely speaking, we have some space, also in this case, for regularizing w_i in such a way that the regularized function is still a critical subsolution, at least on Ω_i .

We can glue together, with some precautions, these regularized local critical subsolutions through a C^∞ partition of the unity, to produce a critical subsolution which is C^∞ outside \mathcal{A} . Using the fact that any critical subsolution is differentiable on \mathcal{A} , we can further adjust the previous construction so that the critical subsolution is C^1 on the whole \mathbb{T}^N . We state this result in the following way: if the equation [1] has a subsolution then it also has a C^1 subsolution. It is worth noticing that it holds even if the underlying manifold is noncompact (see Fathi (2004, 2005b)).

The Intrinsic Lengths and the Action Functional

Here we assume H to satisfy all the usual assumptions in order to define the Hamilton's equations [2]

and to have the completeness of the associated Hamiltonian flow. Namely, we require H to be C^2 in both variables, C^2 -strictly convex, that is, $H_{pp} > 0$ in $\mathbb{T}^N \times \mathbb{R}^N$ and superlinear, in the sense that

$$\lim_{|p| \rightarrow +\infty} \frac{H(x, p)}{|p|} = +\infty \quad \text{uniformly in } x$$

We define the Lagrangian L as the Fenchel transform of H . It takes finite values thanks to the superlinearity condition, and, in addition, inherits, from H , C^2 regularity, C^2 -strict convexity and superlinearity. In our setting, the Fenchel transform is involutive.

We call a vector v_0 and a covector p_0 conjugate at a point x if $v_0 = \bar{H}_p(x, p_0)$, and so $L(x, v_0) = p_0 v_0 - H(x, p_0)$. This also implies the relations $p_0 = L_v(x, v_0)$ and $H(x, p_0) = p_0 v_0 - L(x, v_0)$. If $H(x, p_0) = a$, for some a , then $p_0 v_0 = \sigma_a(x, v_0)$, and p_0 is the unique element of $Z_a(x_0)$ for which such a relation holds. Since the function $y \mapsto p_0 v_0 - H(y, p_0)$ is sub-tangent to $L(\cdot, v_0)$ at x , we see that $L_x(x, v_0) = -H_x(x, p_0)$.

We introduce, for any (Lipschitz-continuous) curve ξ defined in $[a, b]$, for some $a < b$, the action functional $A(\xi)$ through

$$A(\xi) = \int_I L(\xi, \dot{\xi}) \, dt$$

We say that the curve ξ is a minimizer of the action if $A(\xi) \leq A(\gamma)$ for any γ defined $[a, b]$ and with the same end points of ξ . It is a classical result in calculus of variations that any of such minimizers ξ is of class C^2 and satisfies the Euler–Lagrange equation

$$\frac{d}{dt} L_v(\xi, \dot{\xi}) = L_x(\xi, \dot{\xi}) \quad \text{in }]a, b[$$

Consequently, ξ and the conjugate curve $\eta = L_v(\xi, \dot{\xi})$ satisfy the Hamilton's equations [2]. Note that all the integral curves of [2] lie in a fixed level of the Hamiltonian, which is compact by the superlinearity condition. The corresponding Hamiltonian flow is consequently complete.

We show that if $x_0 \in \mathcal{E}$, and $Z_c(x_0) = \{G(x_0)\}$, then $(x_0, G(x_0))$ is a steady state of the Hamiltonian flow. In this case, in fact, $c = \min_p H(x_0, p)$ and so $L(x_0, 0) = -c$ and $H_p(x_0, G(x_0)) = 0$, or equivalently $G(x_0)$ and 0 are conjugate at x_0 . Taking into account that c is the critical value, we have that

$$L(x, 0) = -\min_p H(x, p) \geq -c \quad \text{for any } x \in \mathbb{T}^N$$

so that x_0 is a minimizer of $x \mapsto L(x, 0)$ and $L_x(x_0, 0) = -H_p(x_0, G(x_0)) = 0$. It is easy to see that,

conversely, if (x_0, p_0) is a steady state of the Hamiltonian flow and $H(x_0, p_0) = c$ then $x_0 \in \mathcal{E}$ and $p_0 = G(x_0)$.

We want to establish a relation between $A(\cdot)$ and the length functionals ℓ_a defined in the previous section for $a \geq c$. This will allow, among other things, to show that the Aubry set \mathcal{A} is invariant for the Hamiltonian flow and to analyze the properties of the integral curves lying on it. To this aim, we consider the minimal geodesics for $S_a, a \geq c$, that is, the curves, defined on compact intervals, whose intrinsic lengths ℓ_a equal the distance S_a between their end points.

If $a > c$, we claim that, given any pair of points in \mathbb{T}^N , there is a minimal geodesics joining them. Recalling the formula [12], whose validity depends on the fact that in the strict supercritical case there is a smooth strict subsolution to [1], we have

$$\ell_a(\xi) \rightarrow +\infty \quad \text{whenever} \quad \ell(\xi) \rightarrow +\infty$$

The claim is then proved by using the Ascoli theorem and the lower-semicontinuity property of ℓ_a . In the critical case, given $y \notin \mathcal{A}$, we can use the same argument to deduce the existence of minimizing geodesics for S_c between y and any point x sufficiently close to y (in the Euclidean sense). This comes from the fact that S_c is localizable at y , and so any sequence of curves ξ_n with $\ell_c(\xi_n) \rightarrow S_c(y, x)$ has bounded natural length. For a general pair of points, we will show, on the contrary, that existence of a minimal geodesic is not guaranteed in the critical case.

We consider a minimizing geodesics ξ for S_a between a pair of points y and x . We assume $a > c$ or $a = c$ and $\xi \cap \mathcal{E} = \emptyset$. We want to show that ξ is a minimizing curve for the action, up to a change of parameter. We choose the new parameter in such a way that

$$L(\tilde{\xi}, \dot{\tilde{\xi}}) + a = \sigma_a(\tilde{\xi}, \dot{\tilde{\xi}}) \quad [14]$$

where we have denoted by $\tilde{\xi}$ the reparametrized curve. Since $\tilde{\xi}$ stays away from \mathcal{E} , the velocities $|\dot{\tilde{\xi}}|$ are bounded from below by a positive constant and so the domain of definition of $\tilde{\xi}$, denoted by $[0, T]$, is a compact interval. Note that $\ell_a(\xi) = \ell_a(\tilde{\xi})$, since the intrinsic length is invariant under change of parameter. We take into account that ξ is a minimal geodesic and the inequality $L(x, v) + a \geq \sigma_a(x, v)$, which holds for any x, v , to get

$$A(\tilde{\xi}) = \ell_a(\xi) - aT \leq \ell_a(\gamma) - aT \leq A(\gamma)$$

for any γ defined in $[0, T]$ with $\gamma(0) = y, \gamma(T) = x$. This proves the announced minimality property of $\tilde{\xi}$.

Furthermore, we show that the function $u := S_a(y, \cdot)$ is strictly differentiable at $\tilde{\xi}(s)$, for $s \in]0, T[$, and

$$Du(\tilde{\xi}) = L_v(\tilde{\xi}, \dot{\tilde{\xi}}) =: \eta \quad [15]$$

in $[0, T]$. Hence, $(\tilde{\xi}, Du(\tilde{\xi}))$ is a solution of the Hamilton's equations in $]0, T[$. To see this, we start from the relations

$$\begin{aligned} \int_0^t \frac{d}{ds} u(\tilde{\xi}(s)) ds &= u(\tilde{\xi}(t)) - u(\tilde{\xi}(0)) = \int_0^t \sigma_c(\tilde{\xi}, \dot{\tilde{\xi}}) ds \\ &= \int_0^t \eta \dot{\tilde{\xi}} ds \end{aligned} \quad [16]$$

which hold in $[0, T]$ because u is Lipschitz-continuous, $\tilde{\xi}$ is a minimizing geodesic, and $\eta(s)$ is conjugate to $\dot{\tilde{\xi}}(s)$ at $\tilde{\xi}(s)$ for any $s \in [0, T]$. We know that

$$\begin{aligned} \frac{d}{ds} u(\tilde{\xi}(s)) &= p \dot{\tilde{\xi}}(s) \\ \text{for a.e. } s \text{ and some } p &\in \partial u(\tilde{\xi}(s)) \end{aligned}$$

We have that $p \in Z_c(\tilde{\xi}(s))$, since u is a critical subsolution, and so

$$p \dot{\tilde{\xi}}(s) \leq \sigma_c(\tilde{\xi}(s), \dot{\tilde{\xi}}(s)) = \eta(s) \dot{\tilde{\xi}}(s)$$

We see, in the light of [16], that equality must hold in the previous formula, for a.e. s . Therefore,

$$\frac{d}{ds} u(\tilde{\xi}(s)) = \eta(s) \dot{\tilde{\xi}}(s) \quad \text{for a.e. } s \quad [17]$$

we derive from the fact that the function $\eta(\cdot) \dot{\tilde{\xi}}(\cdot)$ is continuous that $(u(\tilde{\xi}(\cdot)))$ is actually continuously differentiable in $]0, T[$ and that [17] holds for any s . We finally exploit that u is semiconcave in $\mathbb{T}^N \setminus \{y\}$, as pointed out in the previous section, and so $D^+u(\tilde{\xi}(s)) = \partial u(\tilde{\xi}(s))$, for any s . If ϕ is a C^1 -supertangent to u at $\tilde{\xi}(s)$ then

$$D\phi(\tilde{\xi}(s)) \dot{\tilde{\xi}}(s) = \frac{d}{ds} u(\tilde{\xi}(s))$$

accordingly,

$$p \dot{\tilde{\xi}}(s) = \eta(s) \dot{\tilde{\xi}}(s) \quad \text{for any } s \text{ and } p \in \partial u(\tilde{\xi}(s))$$

Since $\partial u(\tilde{\xi}(s)) \subset Z_c(\tilde{\xi}(s))$, this implies that $\partial u(\tilde{\xi}(s)) = \{\eta(s)\}$. This actually gives the strict differentiability function u at $\tilde{\xi}(s)$, and $Du(\tilde{\xi}(s)) = \eta(s)$ for any s .

The same argument works, with some adjustment, also when $a = c$ and $\xi \cap \mathcal{E} \neq \emptyset$. If, for instance, $y \notin \mathcal{E}, t_0 = \min\{t: \xi(t) \in \mathcal{E}\}$, then by reparametrizing ξ in $[0, t_0]$, as indicated in [14], we get a curve $\tilde{\xi}$ defined in $[0, +\infty[$ which is a minimizer of the action functional in any compact interval contained in $[0, +\infty[$. Moreover, $u := S_c(y, \cdot)$ is strictly

differentiable in $]0, +\infty[$ and $(\tilde{\xi}, Du(\tilde{\xi}))$ is a solution of the Hamilton's equations.

We proceed to investigate the properties of the Hamiltonian flow on \mathcal{A} . We take a y_0 in $\mathcal{A} \setminus \mathcal{E}$, and consider a sequence ξ_n of cycles passing through y_0 with $\ell_c(\xi_n) \rightarrow 0$, $\ell(\xi_n) \geq 2\delta$, for some positive δ . Such a sequence does exist in view of the characterization of \mathcal{A} through cycles given in the previous section. Moreover, we assume that the ξ_n are parametrized by the natural arc length in $[-T_n, T_n]$, for some $T_n \geq \delta$, and satisfy $\xi_n(0) = y_0$ for any n . There is then defined a uniform limit curve γ in $[-\delta, \delta]$, up to a subsequence, thanks to the Ascoli theorem.

The idea is to construct a new sequence of cycles γ_n by replacing the portion of the ξ_n between $-\delta$ and δ by γ , and pasting this new piece with the remainder of ξ_n through Euclidean segments at the end points. The γ_n are still of infinitesimal intrinsic length ℓ_c , which shows, in particular, that γ is contained in \mathcal{A} . By exploiting that S_c is a length distance, that the γ_n are cycles, and the formula [7], with $a = c$, we get

$$\begin{aligned} \ell_c(\gamma_n) &\geq S_c(\gamma(-\delta), \gamma(\delta)) + S_c(\gamma(\delta), \gamma(-\delta)) \\ &\geq 0 \end{aligned}$$

for any n , and we at last derive

$$\ell_c(\gamma) = S_c(\gamma(\delta), \gamma(-\delta)) = -S_c(\gamma(-\delta), \gamma(\delta))$$

Note that the second equality is actually redundant. By reparametrizing γ , as in [14], with $a = c$, in some open interval containing 0 as interior point and contained in $[-\delta, \delta]$, we get a curve contained in $\mathcal{A} \setminus \mathcal{E}$, denoted by ξ , defined on some open interval I and satisfying

$$\begin{aligned} A(\xi|_{[s,t]}) + c(t-s) &= \ell_c(\xi|_{[s,t]}) \\ &= -S_c(\xi(t), \xi(s)) \quad \text{for any } t > s \end{aligned} \quad [18]$$

This, in particular, shows that ξ is a minimizer of the action functional in any $[s, t] \subset I$. If we denote, as usual, by η the curve conjugate to ξ , we have, arguing as above, that $\eta(t)$ is the differential of the function $S_c(\xi(s), \cdot)$ at $\xi(t)$, but, since the differentials of all critical subsolutions coincide on \mathcal{A} , we finally get that $\eta(t) = G(\xi(t))$ for every $t \in I$. Therefore, $(\xi, G(\xi))$ is a solution of the Hamilton's equation in I and is contained in $\tilde{\mathcal{A}}$. The same properties can be extended on the whole \mathbb{R} .

Taking into account that if $y \in \mathcal{E}$ then $(y, G(y))$ is a steady state of the Hamiltonian flow, we in the end see that $\tilde{\mathcal{A}}$ is foliated by integral curves of the Hamiltonian flow $(\xi, G(\xi))$, with ξ enjoying the variational property [18]. This is indeed a

characterization since if, conversely, a curve ξ satisfies [18] then it must be contained in \mathcal{A} .

As an application, we finally show that there cannot be minimal geodesics, for the critical metric S_c , joining a point of \mathcal{A} , say y , to some $x \notin \mathcal{A}$, at least when $\mathcal{E} = \emptyset$. If such a geodesic, say ξ , exists, and is defined in $[0, T]$, for some $T > 0$, then $(\xi, Du(\xi))$ is a solution of the Hamilton's equations, up to a change of parameter, where $u := S(y, \cdot)$, satisfying the initial conditions $\xi(0) = y_0$, $\eta(0) = \lim_{t \rightarrow 0^+} Du(\xi(t))$.

The last relation tells us that $\eta(0) \in \partial u(y)$ and, since u is differentiable at $y \in \mathcal{A}$ with $Du(y) = G(y)$, we conclude that $\eta(0) = G(y)$. Therefore, $(\xi, Du(\xi))$ is a part of the integral curve of the Hamiltonian flow starting at $(y, G(y))$ that we know, by the above reasoning, to be contained in \mathcal{A} , which is in contradiction with $\xi(T) = x \notin \mathcal{A}$.

See also: Control Problems in Mathematical Physics; Dynamical Systems in Mathematical Physics: An Illustration from Water Waves; KAM Theory and Celestial Mechanics; Minimax Principle in the Calculus of Variations; Optimal Transportation; Stability Theory and KAM.

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High T_c Superconductor Theory

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Introduction

The phenomenon of superconductivity is one of the most profound manifestations of quantum mechanics in the macroscopic world. The celebrated Bardeen–Cooper–Schrieffer (BCS) theory (Bardeen *et al.* 1957) of superconductivity (SC) provides a basic theoretical framework to understand this remarkable phenomenon in terms of the pairing of electrons with opposite spin and momenta to form a collective condensate state. This theory does not only quantitatively explain the experimental data of conventional superconductors, the basic concepts developed from this theory, including the concept of spontaneous broken symmetry, the Nambu–Goldstone modes and the Anderson–Higgs mechanism provide the essential building blocks for the unified theory of fundamental forces. The discovery of high-temperature superconductivity (HTSC) in the copper oxide material poses a profound challenge to theoretically understand the phenomenon of superconductivity in the extreme limit of strong correlations. While the basic idea of electron pairing in the BCS theory carries over to the HTSC, other aspects like the weak coupling mean field approximation and the phonon mediated pairing mechanism may not apply without modifications. Therefore, HTSC system provides an exciting opportunity to develop new theoretical frameworks and concepts for strongly correlated electronic systems.

To date, a number of different HTSC materials have been discovered. The most studied ones include the hole-doped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_{4+\delta}$ (LSCO), $\text{YBa}_2\text{Cu}_3\text{O}_{6+\delta}$ (YBCO), $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ (BSCO), $\text{Tl}_2\text{Ba}_2\text{CuO}_{6+\delta}$ (TBCO) materials and the electron-doped $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$ (NCCO) material. All these materials have a two-dimensional (2D) CuO_2 plane, and have an antiferromagnetic (AF) insulating phase at half-filling. The magnetic properties of this insulating phase is well approximated by the antiferromagnetic Heisenberg model with spin $S = 1/2$ and an AF exchange constant $J \sim 100$ meV. The Neel temperature for the 3D AF ordering is approximately given by $T_N \sim 300 \sim$

500 K. The HTSC material can be doped either by holes or by electrons. In the doping range of $5\% \lesssim x \lesssim 15\%$, there is an SC phase with a dom-like shape in the temperature versus doping plane. The maximal SC transition temperature T_c is of the order of 100 K. The generic phase diagram of HTSC is shown in Figure 1.

One of the main questions concerning the HTSC phase diagram is the transition region between the AF and the SC phases. Partly because of the complicated material chemistry in this regime, there is no universal agreement among different experiments. Different experiments indicate several different possibilities, including phase separation with an inhomogeneous density distribution, uniform coexistence phase between AF and SC and periodically ordered spin and charge distributions in the form of stripes or checkerboards.

The phase diagram of the HTSC cuprates also contains a regime with anomalous behaviors conventionally called the pseudogap phase. This region of the phase diagram is indicated by the dashed lines in Figure 1. In conventional superconductors, a pairing gap opens up at T_c . In a large class of HTSC cuprates, however, an electronic gap starts to open up at a temperature much higher than T_c . Many experiments indicate that the pseudogap “phase” is

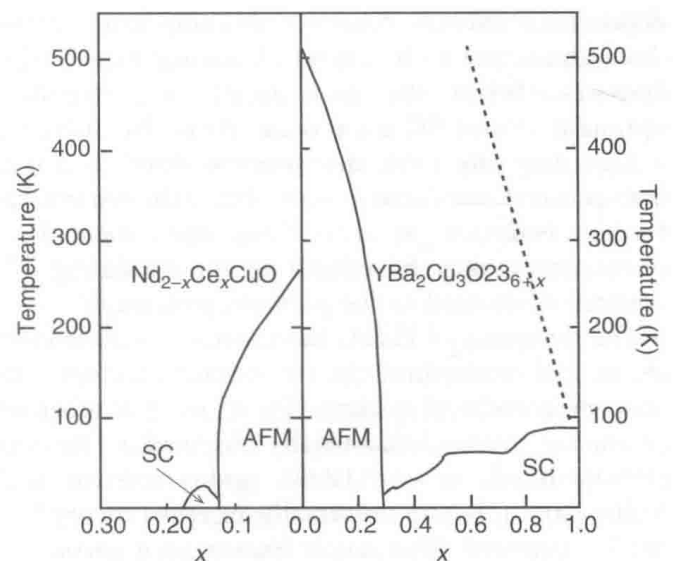


Figure 1 Phase diagram of the of the NCCO and the YBCO superconductors.

not a true thermodynamical phase, but rather the precursor towards a crossover behavior.

The SC phase of the HTSC has a number of striking properties not shared by conventional superconductors. First of all, phase-sensitive experiments indicate that the SC phase for most of the cuprates has d wave like pairing symmetry. This is also supported by the photoemission experiments which show the existence of the nodal points in the quasiparticle gap. Neutron scattering experiments find a new type of collective mode, carrying spin 1, lattice momentum close to (π, π) , and a resolution-limited sharp resonance energy around 20–40 meV. Most remarkably, this resonance mode appears only below T_c of the optimally doped cuprates. Another property uniquely different from the conventional superconductors is the vortex state. Most HTSCs are type II superconductors where the magnetic field can penetrate into the SC state in the form of a vortex lattice, where the SC order is destroyed at the center of the vortex core. In conventional superconductors, the vortex core is filled by the normal metallic electrons. However, a number of different experimental probes, including neutron scattering, muon spin resonance (μ SR), and nuclear magnetic resonance (NMR), have shown that the vortex cores in the HTSC cuprates are antiferromagnetic, rather than normal metallic. This phenomenon has been observed in almost all HTSC materials, including LSCO, YBCO, TBCO, and NSCO, making it one of the most universal properties of the HTSC cuprates.

The HTSC materials also have highly unusual transport properties. While conventional metals have a T^2 dependence of resistivity, in accordance with the predictions of the Fermi liquid theory, the HTSC materials have a linear T dependence of resistivity near optimal doping. This linear T dependence extends over a wide temperature window, and seems to be universal among most of the cuprates. When the underdoped or sometimes optimally doped SC state is destroyed by applying a high magnetic field, the “normal state” is not a conventional conducting state, but exhibits insulator-like behavior, at least along the c -axis. This phenomenon may be related to the insulating AF vortices mentioned in the previous paragraph.

The discovery of HTSC has greatly stimulated the theoretical understanding of superconductivity in strongly correlated systems. There are a number of promising approaches, partially reviewed in Dagotto (1994), Imada *et al.* (1998), and Orenstein and Millis (2000), but an universally accepted theory has not yet emerged. This article focuses on a particular theory, which unifies the AF and the SC phases of the HTSC cuprates based on an approximate SO(5)

symmetry (Zhang 1997). The SO(5) theory draws its inspirations from the successful application of symmetry concepts in theoretical physics. All fundamental laws of Nature are statements about symmetry. Conservation of energy, momentum, and charge are direct consequences of global symmetries. The form of fundamental interactions is dictated by local gauge symmetries. Symmetry unifies apparently different physical phenomena into a common framework. For example, electricity and magnetism were discovered independently, and viewed as completely different phenomena before the nineteenth century. Maxwell’s theory, and the underlying relativistic symmetry between space and time, unify the electric field E and the magnetic field B into a common electromagnetic field tensor $F_{\mu\nu}$. This unification shows that electricity and magnetism share a common microscopic origin, and can be transformed into each other by going to different inertial frames. As discussed previously, the two robust and universal ordered phases of the HTSC are the AF and the SC phases. The central question of HTSC concerns the transition from one phase to the other as the doping level is varied. The SO(5) theory unifies the 3D AF order parameter (N_x, N_y, N_z) and the 2D SC order parameter $(\text{Re}\Delta, \text{Im}\Delta)$ into a single, 5D order parameter called “superspin,” in a way similar to the unification of electricity and magnetism in Maxwell’s theory:

$$F_{\mu\nu} = \begin{pmatrix} 0 & & & \\ E_x & 0 & & \\ E_y & B_z & 0 & \\ E_z & -B_y & B_x & 0 \end{pmatrix} \Leftrightarrow n_a = \begin{pmatrix} \text{Re}\Delta \\ N_x \\ N_y \\ N_z \\ \text{Im}\Delta \end{pmatrix} \quad [1]$$

This unification relies on the postulate that a common microscopic interaction is responsible for both AF and SC in the HTSC cuprates and related materials. A well-defined SO(5) transformation rotates one form of the order into another. Within this framework, the mysterious transition from the AF and the SC as a function of doping is explained in terms of a rotation in the 5D order parameters space. Symmetry principles are not only fundamental and beautiful, they are also practically useful in extracting information from a strongly interacting system, which can be tested quantitatively. The approximate SO(5) symmetry between the AF and the SC phases has many direct consequences, which can be, and some of them have been, tested both numerically and experimentally.

The commonly used microscopic model of the HTSC materials is the repulsive Hubbard model, which describes the electronic degrees of freedom in

the CuO_2 plane. Its low-energy limit, the $t - J$ model is defined by

$$H = -t \sum_{\langle x, x' \rangle} (c_{\sigma}^{\dagger}(x) c_{\sigma}(x') + \text{h.c.}) + J \sum_{\langle x, x' \rangle} \mathbf{S}(x) \cdot \mathbf{S}(x') \quad [2]$$

where the term t describes the hopping of an electron with spin σ from a site x to its nearest neighbor x' , with double occupancy removed, and the J terms describe the nearest-neighbor exchange of its spin \mathbf{S} . The main merit of these models does not lie in the microscopic accuracy and realism, but rather in the conceptual simplicity. However, despite their simplicity, these models are still very difficult to solve, and their phase diagrams cannot be compared directly with experiments. The idea of the $\text{SO}(5)$ theory is to derive an effective quantum Hamiltonian on a coarse-grained lattice, which contains only the superspin degrees of freedom. The resulting $\text{SO}(5)$ quantum nonlinear σ -model is much simpler to solve using the standard field theoretical techniques, and the resulting phase diagram can be compared directly with experiments.

$\text{SO}(4)$ Symmetry of the Hubbard Model

Before presenting the full $\text{SO}(5)$ theory, let us first discuss a much simpler toy model, namely the negative U Hubbard model, which has an SC ground state with s -wave pairing. However, it also has a charge-density-wave (CDW) ground state at half-filling. The competition between CDW and the SC states is similar to the competition between AF and SC states in the HTSC cuprates. In the negative U Hubbard model, the CDW/SC competition can be accurately described by a hidden-symmetry, namely the $\text{SO}(4)$ symmetry of the Hubbard model.

The Hubbard model is defined by the Hamiltonian

$$H = -t \sum_{\langle x, x' \rangle} (c_{\sigma}^{\dagger}(x) c_{\sigma}(x') + \text{h.c.}) + U \sum_x \left(n_{\uparrow}(x) - \frac{1}{2} \right) \left(n_{\downarrow}(x) - \frac{1}{2} \right) - \mu \sum_x n_{\sigma}(x) \quad [3]$$

where $c_{\sigma}(x)$ is the fermion operator and $n_{\sigma}(x) = c_{\sigma}^{\dagger}(x) c_{\sigma}(x)$ is the electron density operator at site x with spin σ , t , U , and μ are the hopping, interaction, and the chemical potential parameters, respectively. The Hubbard model has a pseudospin $\text{SU}(2)$ symmetry generated by the operators

$$\eta^{-} = \sum_x (-)^x c_{\uparrow}(x) c_{\downarrow}(x), \quad \eta^{+} = (\eta^{-})^{\dagger} \\ \eta^z = \frac{1}{2} \sum_{\sigma} \left(n_{\sigma}(x) - \frac{1}{2} \right), \quad [\eta^{\alpha}, \eta^{\beta}] = i \epsilon_{\alpha\beta\gamma} \eta^{\gamma} \quad [4]$$

where $\eta^{\pm} = \eta^x \pm i\eta^y$ and $\alpha = x, y, z$. The model is defined on any bipartite lattice, and the lattice function $(-)^x$ takes the value 1 on even sublattice and -1 on odd sublattice. These operators commute with the Hubbard Hamiltonian at half-filling when $\mu = 0$, that is, $[H, \eta^{\alpha}] = 0$; therefore, they form the symmetry generators of the model (Yang and Zhang 1990). Combined with the standard $\text{SU}(2)$ spin rotational symmetry, the Hubbard model enjoys an $\text{SO}(4) = \text{SU}(2) \otimes \text{SU}(2)/\mathbb{Z}_2$ symmetry. This symmetry has important consequences in the phase diagram and the collective modes in the system. In particular, it implies that the SC and CDW orders are degenerate at half-filling. The SC and the CDW order parameters are defined by

$$\Delta^{-} = \sum_x c_{\uparrow}(x) c_{\downarrow}(x), \quad \Delta^{+} = (\Delta^{-})^{\dagger} \\ \Delta^z = \frac{1}{2} \sum_{x\sigma} (-1)^x n_{\sigma}(x), \quad [\eta^{\alpha}, \Delta^{\beta}] = i \epsilon_{\alpha\beta\gamma} \Delta^{\gamma} \quad [5]$$

where $\Delta^{\pm} = \Delta^x \pm i\Delta^y$. The last equation of [5] shows that the η operators perform the rotation between the SC and CDW order parameters. Thus, η^{α} is the pseudospin generator and Δ^{α} is the pseudospin order parameter. Just like the total spin and the Neel order parameter in the AF Heisenberg model, they are canonically conjugate variables. Since $[H, \eta^{\alpha}] = 0$ at $\mu = 0$, this exact pseudospin symmetry implies the degeneracy of SC and CDW orders at half-filling.

The phase diagram of the $U < 0$ Hubbard model is identical to the phase diagram of the AF Heisenberg model in a uniform magnetic field. If the AF order parameter originally points along the z -direction, a magnetic field applied along the z -direction causes the AF order parameter to flop into the xy -plane. This transition is called the spin-flop transition, and is depicted in **Figures 2a** and **2c**. The chemical potential μ in the negative U Hubbard model plays a role similar to the magnetic field in the AF Heisenberg model. It transforms a CDW state at half-filling to an SC state away from half-filling, as depicted in **Figures 2a** and **2c**.

In the low-energy sector, both the AF Heisenberg model in a magnetic field and the negative- U Hubbard model with a chemical potential can be described by the $\text{SO}(3)$ nonlinear σ -model, which is defined by the following Lagrangian density (in

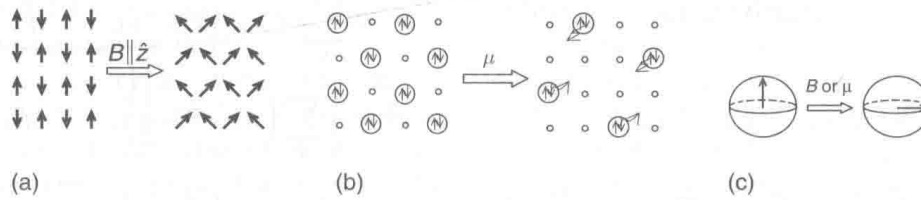


Figure 2 The spin-flop transition. (a) The spin-flop transition of the AF Heisenberg model. When a uniform magnetic field is applied along the direction of the AF moments, there is no net gain of the Zeeman energy. Therefore, after a critical value of the magnetic field, the AF spin component flops into the xy -plane, while a uniform spin component aligns in the direction of applied magnetic field. (b) The Mott insulator to superfluid transition of the hardcore boson model or the $U < 0$ Hubbard model. At half-filling, one possible state is the CDW state of ordered boson pairs. Upon doping, the pairs become mobile and form the superfluid state. (c) Both transitions can be described by the spin or the pseudospin flop in the $SO(3)$ nonlinear σ -model, induced either by the magnetic field or by the chemical potential.

imaginary time coordinates) for a unit vector field n_α with $n_\alpha^2 = 1$:

$$\mathcal{L} = \frac{\chi}{2} \omega_{\alpha\beta}^2 + \frac{\rho}{2} (\partial_t n_\alpha)^2 + V(n) \quad [6]$$

$$\omega_{\alpha\beta} = n_\alpha (\partial_t n_\beta - i B_{\beta\gamma} n_\gamma) - (\alpha \rightarrow \beta)$$

where the magnetic field, or equivalently the chemical potential, is given by $B_\alpha = (1/2)\epsilon_{\alpha\beta\gamma} B_{\beta\gamma}$. χ and ρ are the susceptibility and stiffness parameters, and $V(n)$ is the anisotropy potential, which can be taken as $V(n) = -(g/2)n_z^2$. Exact $SO(3)$ symmetry is obtained when $g = B_\alpha = 0$. $g > 0$ corresponds to easy axis anisotropy, while $g < 0$ corresponds to easy plane anisotropy. In the case of $g > 0$, there is a phase transition as a function of B_z with $B_x = B_y = 0$. To see this, let us expand out the first term in [6]. The time-independent part contributes to an effective potential

$$V_{\text{eff}} = V(n) - \frac{\chi B^2}{2} (n_x^2 + n_y^2)$$

from which we see that there is a phase transition at $B_{c1} = \sqrt{g/\chi}$. For $B < B_{c1}$, the system is in the Ising phase, while for $B > B_{c1}$, the system is in the XY phase. Therefore, tuning B for a fixed $g > 0$ leads to the spin-flop transition. In $D=2$, both the XY and the Ising phase can have a finite-temperature phase transition into the disordered state. However, because of the Mermin–Wagner theorem, a finite-temperature phase transition is forbidden at the point $B = g = 0$, where the system has an enhanced $SO(3)$ symmetry. This $SO(3)$ symmetric point leads to a large regime below the mean field transition temperature where the fluctuation dominates. This large fluctuation regime can be identified as the pseudogap behavior.

The pseudospin $SU(2)$ symmetry of the negative- U Hubbard model has another important consequence. Away from half-filling, the η operators no longer commute with the Hamiltonian, but they are eigenoperators of the Hamiltonian, in the sense that

$$[H, \eta^\pm] = \mp 2\mu \eta^\pm \quad [7]$$

This means that the η operators create well-defined collective modes with energy 2μ . Since they carry charge ± 2 , they usually do not couple to any physical probes. However, in an SC state, the SC order parameter mixes the η operators with the CDW operator Δ^z , via eqn [5]. From this reasoning, a pseudo-Goldstone mode was predicted to exist in the density response function at wave vector (π, π) and energy 2μ , which appears only below the SC transition temperature T_c .

Unification of Antiferromagnetism and Superconductivity through the $SO(5)$ Theory

Order Parameters and $SO(5)$ Group Properties

The negative U Hubbard model and the $SO(3)$ nonlinear σ -models discussed in the previous section give a nice description of the quantum phase transition from the Mott insulating phase with CDW order to the SC phase. On the other hand, these simple models do not have enough complexity to describe the AF insulator at half-filling and the SC order away from half-filling. Therefore, a natural step is to generalize these models so that the Mott insulating phase with the scalar CDW order parameter is replaced by a Mott insulating phase with the vector AF order parameter. The pseudospin $SO(3)$ symmetry group considered previously arises from the combination of one real scalar component of the CDW order parameter with one complex, or two real components of the SC order parameter. After replacing the scalar CDW order parameter by the three components of the AF order parameter, and combining with the two components of the SC order parameters, we are naturally led to consider a five-component order parameter vector, and the $SO(5)$ symmetry group which transforms it.

It is simplest to define the concept of the $SO(5)$ symmetry generator and order parameter on two sites with fermion operators c_σ and d_σ , respectively,

where $\sigma = 1, 2$ is the usual spin index. The AF order parameter operator can be naturally defined in terms of the difference between the spins of the c and d fermions as follows:

$$N^\alpha = \frac{1}{2}(c^\dagger \tau^\alpha c - d^\dagger \tau^\alpha d), \quad n_2 \equiv N_1 \quad [8]$$

$$n_3 \equiv N_2, \quad n_4 \equiv N_3$$

where τ^α are the Pauli matrices. In view of the strong on-site repulsion in the cuprate problem, the SC order parameter should be naturally defined on a bond connecting the c and d fermions, explicitly given by

$$\Delta^\dagger = \frac{-i}{2} c^\dagger \tau^y d^\dagger = \frac{1}{2} (-c^\dagger_\uparrow d^\dagger_\downarrow + c^\dagger_\downarrow d^\dagger_\uparrow), \quad [9]$$

$$n_1 \equiv \frac{(\Delta^\dagger + \Delta)}{2}, \quad n_5 \equiv \frac{(\Delta^\dagger - \Delta)}{2i}$$

We can group these five components together to form a single vector $n_a = (n_1, n_2, n_3, n_4, n_5)$ called the superspin, since it contains both superconducting and antiferromagnetic spin components. The individual components of the superspin are explicitly defined in the last parts of eqns [8] and [9].

The concept of the superspin is only useful if there is a natural symmetry group acting on it. In this case, since the order parameter is 5D, it is natural to consider the most general rotation in the 5D order parameter space spanned by n_a . In 3D, three Euler angles specify a general rotation. In higher dimensions, a rotation is specified by selecting a plane and the angle of rotation within this plane. Since there are $n(n-1)/2$ independent planes in n dimensions, the group $SO(n)$ is generated by $n(n-1)/2$ elements, specified in general by antisymmetric matrices $L_{ab} = -L_{ba}$, with $a = 1, \dots, n$. In particular, the $SO(5)$ group has ten generators. The total spin and the total charge operator

$$S_\alpha = \frac{1}{2}(c^\dagger \tau_\alpha c + d^\dagger \tau_\alpha d) \quad [10]$$

$$Q = \frac{1}{2}(c^\dagger c + d^\dagger d - 2)$$

perform the function of rotating the AF and SC order parameters within each subspace. In addition, there are six so-called π operators, defined by

$$\pi^\dagger_\alpha = -\frac{1}{2} c^\dagger \tau_\alpha \tau_y d^\dagger, \quad \pi_\alpha = (\pi^\dagger_\alpha)^\dagger \quad [11]$$

which perform the rotation from AF to SC and vice versa. These infinitesimal rotations are defined by the commutation relations

$$[\pi^\dagger_\alpha, N_\beta] = i\delta_{\alpha\beta} \Delta^\dagger, \quad [\pi^\dagger_\alpha, \Delta] = iN_\alpha \quad [12]$$

The ten operators, the total spin S_α , the total charge Q , and the six π operators form the ten generators of the $SO(5)$ group.

The superspin order parameter n_a , the associated $SO(5)$ generators L_{ab} , and their commutation relations can be expressed compactly and elegantly in terms of the $SO(5)$ spinor and the five Dirac Γ matrices. The four-component $SO(5)$ spinor is defined by

$$\Psi_\mu = \begin{pmatrix} c_\sigma \\ d^\dagger_\sigma \end{pmatrix} \quad [13]$$

They satisfy the usual anticommutation relations

$$\{\Psi^\dagger_\mu, \Psi_\nu\} = \delta_{\mu\nu}, \quad \{\Psi_\mu, \Psi_\nu\} = \{\Psi^\dagger_\mu, \Psi^\dagger_\nu\} = 0 \quad [14]$$

Using the Ψ spinor and the five Dirac Γ matrices, we can express n_a and L_{ab} as

$$n_a = \frac{1}{2} \Psi^\dagger_\mu \Gamma^a_{\mu\nu} \Psi_\nu, \quad L_{ab} = -\frac{1}{2} \Psi^\dagger_\mu \Gamma^{ab}_{\mu\nu} \Psi_\nu \quad [15]$$

The L_{ab} operators satisfy the commutation relation

$$[L_{ab}, L_{cd}] = -i(\delta_{ac} L_{bd} + \delta_{bd} L_{ac} - \delta_{ad} L_{bc} - \delta_{bc} L_{ad}) \quad [16]$$

The n_a and the Ψ_μ operators form the vector and the spinor representations of the $SO(5)$ group, satisfying the following equations:

$$[L_{ab}, n_c] = -i(\delta_{ac} n_b - \delta_{bc} n_a) \quad [17]$$

and

$$[L_{ab}, \Psi_\mu] = -\frac{1}{2} \Gamma^{ab}_{\mu\nu} \Psi_\nu \quad [18]$$

If we arrange the ten operators S_α, Q , and π_α into L_{ab} 's by the following matrix form:

$$L_{ab} = \begin{pmatrix} 0 & & & & \\ \pi^\dagger_x + \pi_x & 0 & & & \\ \pi^\dagger_y + \pi_y & -S_z & 0 & & \\ \pi^\dagger_z + \pi_z & S_y & -S_x & 0 & \\ Q & \frac{1}{i}(\pi^\dagger_x - \pi_x) & \frac{1}{i}(\pi^\dagger_y - \pi_y) & \frac{1}{i}(\pi^\dagger_z - \pi_z) & 0 \end{pmatrix} \quad [19]$$

and group n_a as in eqns [8] and [9], we see that eqns [16] and [17] compactly reproduce all the commutation relations worked out previously. These equations show that L_{ab} and n_a are the symmetry generators and the order parameter vectors of the $SO(5)$ theory.

Having introduced the concept of local symmetry generators and order-parameter-based sites in real space, we now proceed to discuss definitions of these operators in momentum space. The AF and dSC order parameters can be naturally expressed in terms of the microscopic fermion operators as

$$N^\alpha = \sum_p c^\dagger_{p+\Pi} \tau^\alpha c_p, \quad \Delta^\dagger = \frac{-i}{2} \sum_p d(p) c^\dagger_p \tau^y c^\dagger_{-p} \quad [20]$$

$$d(p) \equiv \cos p_x - \cos p_y$$

where $\Pi \equiv (\pi, \pi)$ and $d(p)$ is the form factor for d -wave pairing in 2D. They can be combined into the five-component superspin vector n_a by using the

Table 1 Quantum number of the AF and the dSC order parameters, and the π operator, which rotates the AF and the dSC order parameters into each other

	Charge	Spin	Momentum	Internal angular momentum
Δ, Δ^\dagger or n_1, n_5	± 2	0	0	d-Wave
N^α or $n_{2,3,4}$	0	1	(π, π)	s-Wave
$\pi_\alpha, \pi_\alpha^\dagger$	± 2	1	(π, π)	d-Wave

same convention as before. The total spin and total charge operator are defined microscopically as

$$S_\alpha = \sum_p c_p^\dagger \tau^\alpha c_p, \quad Q = \frac{1}{2} \sum_p (c_p^\dagger c_p - 1) \quad [21]$$

and the π -operators can be defined as

$$\pi_\alpha^\dagger = \sum_p g(p) c_{p+\Pi}^\dagger \tau^\alpha \tau^y c_{-p}^\dagger \quad [22]$$

The form factor $g(p)$ needs to be chosen appropriately to satisfy the SO(5) commutation relation [16], and this requirement determines $g(p) = \text{sgn}(d(p))$.

The SO(5) symmetry generators perform the most general rotation among the five-order parameters. It is easy to see that the quantum number of the π operators exactly patches up the difference in quantum numbers between the AF and the dSC order parameters, according to Table 1.

The SO(5) quantum nonlinear σ -model

In the previous section we presented the concept of the local SO(5) order parameters and symmetry generators. These relationships are purely kinematic, and do not refer to any particular Hamiltonian. One can in fact construct microscopic models with exact SO(5) symmetry out of these operators. A large class of models, however, may not have SO(5) symmetry at the microscopic level, but their long-distance, low-energy properties may be described in terms of an effective SO(5) model. In the previous section, we have seen that many different microscopic models indeed all have the SO(3) nonlinear σ -model as their universal low-energy description. Similarly, we present the SO(5) quantum nonlinear σ -model as a general theory of AF and dSC in the HTSC.

From eqn [17] and the discussions in the previous subsection, we see that L_{ab} and n_a are conjugate degrees of freedom, very much similar to $[q, p] = i\hbar$ in quantum mechanics. This suggests that we can construct a Hamiltonian from these conjugate degrees of freedom. The Hamiltonian of the SO(5)

quantum nonlinear σ -model takes the following form:

$$H = \frac{1}{2\chi} \sum_x L_{ab}^2(x) + \frac{\rho}{2} \sum_{\langle x, x' \rangle} n_a(x) n_a(x') + \sum_x B_{ab}(x) L_{ab}(x) + \sum_x V(n(x)) \quad [23]$$

where the n_a vector field is subjected to the constraint

$$n_a^2 = 1 \quad [24]$$

This Hamiltonian is quantized by the canonical commutation relations [16] and [17]. Here, the first term is the kinetic energy of the SO(5) rotors, where χ has the physical interpretation of the moment of inertia of the SO(5) rotors. The second term describes the coupling of the SO(5) rotors on different sites, through the generalized stiffness ρ . The third term introduces the coupling of external fields to the symmetry generators, while the $V(n)$ can include anisotropic terms to break the SO(5) symmetry to the SO(3) \times U(1) symmetry. The SO(5) quantum nonlinear σ -model is a natural combination of the SO(3) nonlinear σ -model describing the AF Heisenberg model and the quantum XY model describing the SC to insulator transition. If we restrict to the values $a=2, 3, 4$, then the first two terms describe the symmetric Heisenberg model, the third term describes easy plane or easy axis anisotropy of the Neel vector, while the last term represents the coupling to the uniform external magnetic field. On the other hand, for $a=1, 5$, the first term describes Coulomb or capacitance energy, the second term is the Josephson coupling energy, while the last term describes coupling to external chemical potential.

The first two terms of the SO(5) model describe the competition between the quantum disorder and classical order. In the ordered state, the last two terms describe the competition between the AF and the SC order. Let us first consider the quantum competition. The first term prefers sharp eigenstates of the angular momentum. At an isolated site, $C \equiv \sum L_{ab}^2$ is the Casimir operator of the SO(5) group, in the sense that it commutes with all the SO(5) generators. The eigenvalues of this operator can be determined completely from group theory; they are 0, 4, 6, and 10, respectively, for the 1D SO(5) singlet, 5D SO(5) vector, 10D antisymmetric tensor, and 14D symmetric, traceless tensors. Therefore, we see that this term always prefers a quantum-disordered SO(5) singlet ground state, which is a total spin singlet. This ground state is separated from the first excited state, the fivefold

SO(5) vector state with an energy gap of $2/\chi$. This gap will be reduced, when the different SO(5) rotors are coupled to each other by the second term. This term represents the effect of stiffness, which prefers a fixed direction of the n_a vector, rather than a fixed angular momentum. This competition is an appropriate generalization of the competition between the number sharp and phase sharp states in a superconductor and the competition between the classical Neel state and the bond or plaquette singlet state in the Heisenberg AF. The quantum phase transition occurs near $\chi\rho \simeq 1$.

In the classically ordered state, the last two anisotropy terms compete to select a ground state. To simplify the discussion, we can first consider the following simple form of the static anisotropy potential:

$$V(n) = -g(n_2^2 + n_3^2 + n_4^2) \quad [25]$$

At the particle-hole symmetric point with vanishing chemical potential $B_{15} = \mu = 0$, the AF ground state is selected by $g > 0$, while the SC ground state is selected by $g < 0$ coupled with the constraint $n_a^2 = 1$. $g = 0$ is the quantum phase transition point separating the two ordered phases.

However, it is unlikely that the HTSC cuprates can be close to this quantum phase transition point. In fact, we expect the anisotropy term g to be large and positive, so that the AF phase is strongly favored over the SC phase at half-filling. However, the chemical potential term has the opposite, competing effect favoring SC. To see this, we transform the Hamiltonian into the Lagrangian density (in imaginary time coordinates) in the continuum limit:

$$\mathcal{L} = \frac{\chi}{2} \omega_{ab}(x, t)^2 + \frac{\rho}{2} (\partial_k n^a(x, t))^2 + V(n(x, t)) \quad [26]$$

where

$$\omega_{ab} = n_a(\partial_t n_b - iB_{bc}n_c) - (a \rightarrow b) \quad [27]$$

is the angular velocity. We see that the chemical potential enters the Lagrangian as a gauge coupling in the time direction. Expanding the time derivative term, we obtain an effective potential

$$V_{\text{eff}}(n) = V(n) - \frac{(2\mu)^2 \chi}{2} (n_1^2 + n_5^2) \quad [28]$$

from which we see that the V term competes with the chemical potential term. For $\mu < \mu_c = \sqrt{g/\chi}$, the AF ground state is selected, while for $\mu > \mu_c$, the SC ground state is realized. At the transition point, even though each term strongly breaks SO(5) symmetry, the combined term gives an effective static potential which is SO(5) symmetric, as we can see from [28].

Even though the static potential is SO(5) symmetric, the full quantum dynamics is not. This can be most easily seen from the time-dependent term in the Lagrangian. When we expand out the square, the term quadratic in μ enters the effective static potential in eqn [28]. However, there is also a time-dependent term linear in μ . This term breaks the particle-hole symmetry, and it dominates over the second-order time derivative term in the n_1 and n_5 variables. In the absence of an external magnetic field, only second-order time derivative terms of $n_{2,3,4}$ enter the Lagrangian. Therefore, while the chemical potential term compensates the anisotropy potential in eqn [28] to arrive at an SO(5) symmetric static potential, its time-dependent part breaks the full quantum SO(5) symmetry. This observation leads to the concept of the projected, or static SO(5) symmetry (Zhang *et al.* 1999). A model with projected or static SO(5) symmetry is described by a quantum effective Lagrangian of the form

$$\mathcal{L} = \frac{\chi}{2} \sum_{a=2,3,4} (\partial_t n_a)^2 - \chi \mu (n_1 \partial_t n_5 - n_5 \partial_t n_1) - V_{\text{eff}}(n) \quad [29]$$

where the static potential V_{eff} is SO(5) symmetric, but the time-dependent part contains a first-order time derivative term in n_1 and n_5 .

The SO(5) quantum nonlinear σ -model is constructed from two canonically conjugate field operators L_{ab} and n_a . In fact, there is a kinematic constraint among these field operators:

$$L_{ab}n_c + L_{bc}n_a + L_{ca}n_b = 0 \quad [30]$$

This identity is valid for any triples a, b , and c , and can be easily proved by expressing $L_{ab} = n_a p_b - n_b p_a$, where p_a is the conjugate momentum of n_a . Geometrically, this identity expresses the fact that L_{ab} generates a rotation of the n_a vector. The infinitesimal rotation vector lies on the tangent plane of the four sphere S^4 , and is therefore orthogonal to the n_a vector itself.

In a large class of materials, including the high- T_c cuprates, the organic superconductors, and the heavy fermion compounds, the AF and SC phases occur in close proximity to each other. The SO(5) theory is developed based on the assumption that these two phases share a common microscopic origin and should be treated on an equal footing. The SO(5) theory gives a coherent description of the rich global phase diagram of the high- T_c cuprates and its low-energy dynamics through a simple symmetry principle and a unified effective model based on a single quantum Hamiltonian. A number of theoretical predictions, including the intensity dependence of the neutron resonance

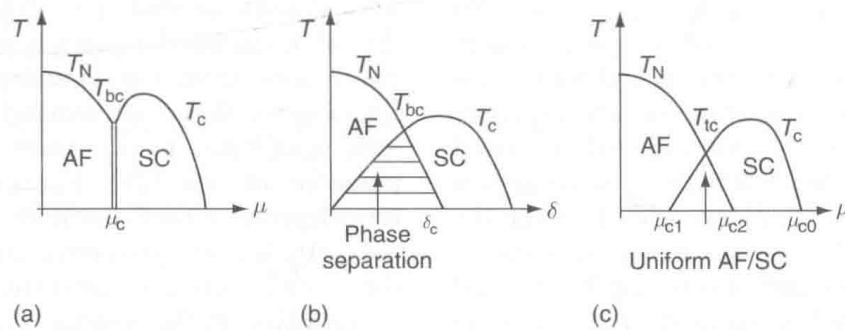


Figure 3 The finite-temperature phase diagram of the SO(5) model in the temperature (T) versus chemical potential (μ) plane. (a) and (b) are two different representations of the same phase diagram, corresponding to a direct first-order phase transition between AF and SC, as a function of the chemical potential and doping, respectively. (c) corresponds to two second-order phase transitions with a uniform AF/SC mix phase in between. The AF and the SC transition temperatures T_N and T_c merge into a bicritical T_{bc} or a tetra-critical point T_{tc} . Both possibilities are allowed theoretically; it is up to experiments to determine which one is actually realized in the high- T_c cuprates.

mode, the AF vortex state, and the mixed phase of AF and SC, have been verified experimentally (Figure 3). The theory also sheds light on the microscopic mechanism of superconductivity and quantitatively correlates the AF exchange energy with the condensation energy of superconductivity. However, the theory is still incomplete in many ways and lacks full quantitative predictive power. While the role of fermions is well understood within the exact SO(5) models, their roles in the effective SO(5) models are still not fully worked out. As a result, the theory has not made many predictions concerning the transport properties of these materials.

See also: Abelian Higgs Vortices; Effective Field Theories; Euclidean Field Theory; Ginzburg–Landau Equation; Hubbard Model; Quantum Phase Transitions; Quantum Spin Systems; Quantum Statistical Mechanics:

Overview; Renormalization: General Theory; Renormalization: Statistical Mechanics and Condensed Matter; Superfluids; Symmetry Classes in Random Matrix Theory; Variational Techniques for Ginzburg–Landau Energies.

Further Reading

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Holomorphic Dynamics

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Introduction

Subject

Holomorphic dynamics (in a narrow sense) is a theory of iterates of rational endomorphisms of the Riemann sphere $\hat{\mathbb{C}} = \mathbb{C} \cup \{\infty\}$. The goal is to understand the *phase portrait* of this dynamical system, that is, the structure of its trajectories, and the dependence of the phase portrait on *parameters* (coefficients of f).

Holomorphic dynamics in a broader sense would include the theory of analytic transformations, local and global, in dimension 1 and higher, as well as the theory of groups and pseudogroups of analytic transformations, which would cover theory of Kleinian groups and holomorphic foliations. However, we will mostly focus on holomorphic dynamics in the narrow sense.

Brief History

Local dynamical theory of analytic maps was laid down in the late nineteenth and early twentieth century by Königs, Schröder, Böttcher, and Leau. Global theory of iterates of rational maps was founded by Fatou and Julia in comprehensive memoirs of 1918–19. The theory had been

developed very little since then until early 1980s when it exploded with new methods, ideas, and computer images. Particularly influential were the works of D Sullivan who introduced ideas of *quasiconformal deformations* into the field, of A Douady and J Hubbard who gave a comprehensive combinatorial description of the Mandelbrot set, and W Thurston who linked holomorphic dynamics to three-dimensional hyperbolic geometry bringing to the field ideas of geometrization and rigidity. As a result, profound rigidity conjectures were formulated. Renormalization ideas introduced to the theory later on led to a significant progress towards these conjectures (see Universality and Renormalization).

Another source of ideas came from ergodic theory and the general theory of dynamical systems, particularly hyperbolic dynamics and thermodynamical formalism. They led to constructions of natural geometric measures on the Julia sets that helped to penetrate into their fractal nature.

General Terminology and Notations

$\mathbb{N} = \{1, 2, \dots\}$ is the set of natural numbers; \mathbb{D} is the unit disk; $\mathbb{Z}_+ = \mathbb{N} \cup \{0\}$; $\mathbb{T} = \partial\mathbb{D}$.

A *topological disk* is a simply connected domain in \mathbb{C} . A *topological annulus* is a doubly connected domain in \mathbb{C} (i.e., a domain homeomorphic to a round annulus). A *Cantor set* is a totally disconnect compact subset of \mathbb{R}^n without isolated points.

Given a map $f: X \rightarrow X$, f^n will stand for its n -fold iterate. The semigroup of iterates form a *dynamical system with discrete time*. An *orbit* or *trajectory* of a point z is $\text{orb}_f(z) = (f^n z)_{n=0}^\infty$.

A subset $Y \subset \hat{\mathbb{C}}$ is called *invariant* if $f(Y) \subset Y$ and *completely invariant* if also $f^{-1}(Y) \subset Y$.

A point $\alpha \in \hat{\mathbb{C}}$ is called *periodic* if $f^p \alpha = \alpha$ for some natural p . The smallest such p is called the *period* of α . If $p=1$, then α is called a *fixed point*. The orbit of a periodic point is also called a *cycle*.

Two maps $f: X \rightarrow X$ and $g: Y \rightarrow Y$ on topological spaces X and Y are called *topologically conjugate* if there exists a homeomorphism $h: X \rightarrow Y$ such that $h \circ f = g \circ h$. If h has better regularity properties, for example, it is quasiconformal/conformal/affine, then f and g are called *quasiconformally/conformally/affinely conjugate*.

Let $f(z) = P(z)/Q(z)$ be a rational function viewed as a map $\hat{\mathbb{C}} \rightarrow \hat{\mathbb{C}}$. Its *topological degree* $\deg f = \#f^{-1}(z)$, $z \in \hat{\mathbb{C}}$, (where the preimages of z are counted with multiplicity), is equal to the *algebraic degree* $\max(\deg P, \deg Q)$. The dynamics of f is very

simple in degree 1, so in what follows we assume that $\deg f \geq 2$.

Let $C_f = \{c: Df(c) = 0\}$ stand for the set of *critical points* of f , and $V_f = f(C_f)$ be the set of *critical values*. A rational function of degree d has $2d - 2$ critical points counted with multiplicity. Moreover,

$$C_{f^n} = \bigcup_{k=0}^{n-1} f^{-k}(C_f), \quad V_{f^n} = \bigcup_{k=1}^n f^k(C_f)$$

The latter formula explains why the behavior of the critical orbits crucially influences the global dynamics of f . The set $O_f = \bigcup V_{f^n}$ is called *postcritical*.

Basic Dynamical Theory

Local Theory

The local theory describes the dynamics of an analytic map $f: z \mapsto \lambda z + \sum_{n=2}^\infty a_n z^n$ near its fixed point 0. The derivative $\lambda = f'(0)$ is called the multiplier of 0. The fixed point is called *attracting*, *repelling*, or *neutral*, depending on whether $|\lambda| < 1$, $|\lambda| > 1$, or $|\lambda| = 1$. It is called *superattracting* if $\lambda = 0$.

In case when 0 is an attracting (but not superattracting) or repelling fixed point, the map is *linearizable*, that is, it is conformally conjugate to its linear part $z \mapsto \lambda z$; thus, there is a local conformal solution of the *Schröder equation* $\phi(fz) = \lambda \phi(z)$. This solution is also called the *linearizing coordinate* near 0.

In the superattracting case, the map is conformally conjugate to the map $z \mapsto z^d$, where $a_d z^d$ is the first nonvanishing term in the local expansion of f . Thus, in this case there is a local conformal solution of the *Böttcher equation* $\phi(fz) = \phi(z)^d$. It is also called the *Böttcher coordinate* near 0.

The situation in the neutral case (when $\lambda = e^{2\pi i \theta}$, $\theta \in \mathbb{R}/\mathbb{Z}$) depends in a delicate way on the arithmetic properties of the *rotation number* θ . If $\theta = q/p$ is rational, the fixed point 0 is called *parabolic*. The local dynamics is then described in terms of the *Leau-Fatou flower* consisting of attracting petals alternating with repelling petals. In each petal, the map is conformally conjugate to the translation $z \mapsto z + 1$. The quotients of the petals by dynamics are conformally equivalent to the cylinder $\mathbb{C}/\langle z \mapsto z + 1 \rangle$. They are called (*attracting/repelling*) *Ecalé-Voronin cylinders*.

In the *irrational* case, when $\theta \in \mathbb{R} \setminus \mathbb{Q}$, the map can be either linearizable or not. Accordingly, 0 is called a *Siegel* or a *Cremer* fixed point. If the multiplier is *Diophantine* (i.e., there exist $C > 0$ and $\alpha > 2$ such that for all rational numbers q/p , we have: $|\theta - q/p| \geq Cp^\alpha$), then 0 is linearizable (Siegel 1942).

Notice that almost all numbers are Diophantine. A sharper arithmetic condition for linearizability in terms of the continuous fraction expansion for θ was given by Bruno (1965). In the quadratic case, $z \mapsto e^{2\pi i\theta}z + z^2$, this condition was proved to be sharp (Yoccoz 1988).

Fatou and Julia Sets

From now on, $f: \hat{\mathbb{C}} \rightarrow \hat{\mathbb{C}}$ is a rational endomorphism of the Riemann sphere. The theory starts with the splitting of the sphere into two subsets now called Fatou and Julia sets based on the notion of a normal family in the sense of Montel. A family $(\phi_\alpha: S \rightarrow \hat{\mathbb{C}})$ of meromorphic functions on some Riemann surface S is called *normal* if it is precompact in the open-closed topology. The *Fatou set* $F(f)$ is the maximal open subset of $\hat{\mathbb{C}}$ on which the family of iterates $(f^n)_{n=0}^\infty$ is normal. The *Julia set* $J(f)$ is the complement of the Fatou set. Both sets are completely invariant. The Julia set is always nonempty, and is either nowhere dense or coincides with the whole sphere. The trajectories on the Fatou set are *Lyapunov stable* (if z is close to $z_0 \in F(f)$, then $\text{orb}_f(z)$ is uniformly close to $\text{orb}_f(z_0)$), while the dynamics on the Julia set is “chaotic.”

If f is a polynomial, then the Fatou and Julia sets can be defined in a more concrete way as follows. In this case, ∞ is a superattracting fixed point for f . Let us consider its *basin of attraction*,

$$D_f(\infty) = \{z: f^n z \rightarrow \infty \text{ as } n \rightarrow \infty\}$$

Its complement, $K(f)$, is called the *filled Julia set*. Then,

$$J(f) = \partial K(f) = \partial D_f(\infty)$$

Periodic Points

Let α be a periodic point of f of period p . As a fixed point of f^p , it is subject of the local theory. Thus, it (and its cycle) is classified as *attracting*, *repelling*, etc., according to the properties of the *multiplier* $\lambda = (f^p)'(\alpha)$ (that can be calculated in any local chart near α).

The *basin of attraction* $D_f(\alpha)$ of an attracting cycle $\alpha = (f^n \alpha)_{n=0}^{p-1}$ is the set $\{z: f^n z \rightarrow \alpha \text{ as } n \rightarrow \infty\}$. The *immediate basin of attraction* $D_f^*(\alpha)$ is the union of components of $D_f(\alpha)$ containing the points of α .

Theorem 1 (Fatou–Julia). *The immediate basin of any attracting cycle contains a critical point. (Note that a superattracting cycle actually contains some critical point.)*

It follows that a rational function of degree d has at most $2d - 2$ attracting cycles. A polynomial of degree d has at most $d - 1$ attracting cycles in \mathbb{C} .

Attracting cycles belong to the Fatou set, while repelling cycles lie on the Julia set. Parabolic and Cremer points lie on the Julia set, while Siegel points belong to the Fatou set. The *basin of attraction* of a parabolic cycle α is defined as

$$D_f(\alpha) = \{z: f^n z \rightarrow \alpha \text{ as } n \rightarrow \infty\} \setminus \bigcup_{n=0}^{\infty} f^{-n}(\alpha)$$

It is the union of some components of the Fatou set. The union of the components of $D_f(\alpha)$ containing the petals of the Leau–Fatou flower is called the *immediate basin of attraction* $D_f^*(\alpha)$ of α . As in the attracting case, the immediate basin $D_f^*(\alpha)$ of a parabolic cycle contains a critical point of f .

Components of the Fatou set containing Siegel periodic points are called *Siegel disks*. If D is a Siegel disk of period p , then $f^p|_D$ is conformally conjugate to the irrational rotation $z \mapsto e^{2\pi i\theta}z$ of the unit disk.

Theorem 2 (Shishikura 1987). *A rational function of degree d has at most $2d - 2$ nonrepelling cycles.*

The proof of this result uses the methods of quasiconformal surgery.

Examples

For $f: z \mapsto z^d$, $d \geq 2$, the Julia set $J(f)$ is the unit circle. Moreover, $D_f(\infty) = \hat{\mathbb{C}} \setminus \bar{D}$, while D is the basin of attraction of the superattracting fixed point 0.

For maps $f_\varepsilon: z \mapsto z^2 + \varepsilon$ with sufficiently small $\varepsilon \neq 0$, the Julia set $J(f)$ is a *nowhere-differentiable* Jordan curve (see Figure 1). The domain bounded by this curve is the basin of attraction of an attracting fixed point α_ε .

The filled Julia set of the map $f: z \mapsto z^2 - 1$ called the *basilica* is depicted in black in Figure 2. The

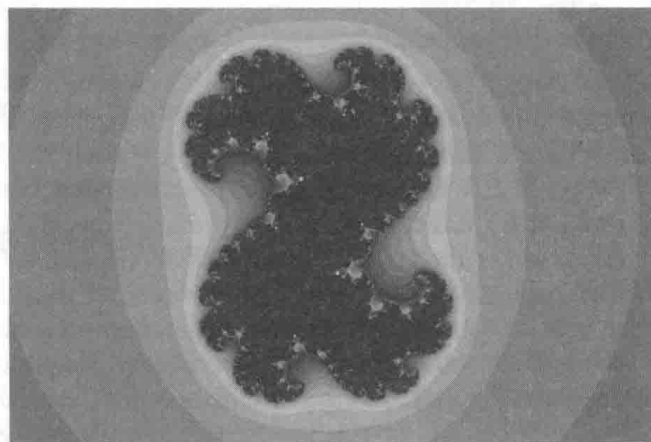


Figure 1 Nowhere-differentiable Jordan curve.

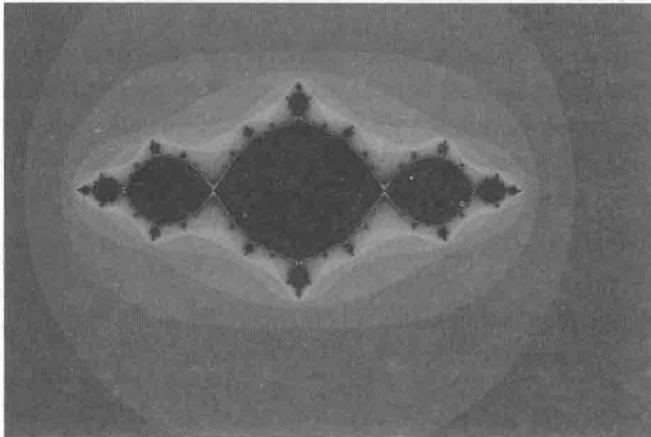


Figure 2 Basilica.

interior of the basilica is the basin of the super-attracting cycle $\alpha = (0, 1)$ of period 2.

For the map $f: z \mapsto z^2 - 2$, the Julia set is the interval $[-2, 2]$. It is affinely conjugate to the Chebyshev quadratic polynomial $Ch_2: z \mapsto 2z^2 - 1$. More generally, for a Chebyshev polynomial Ch_d of any degree d , the Julia set is the interval. (By definition, the Chebyshev polynomial Ch_d is the solution of the functional equation $\cos dz = Ch_d(\cos z)$.)

For quadratic maps $f_c: z \mapsto z^2 + c$ with $c < -2$, the Julia set is a Cantor set on \mathbb{R} . For maps f_c with $c > 1/4$, the Julia set is a Cantor set that does not meet \mathbb{R} . For $c \in (-2, 1/4]$, the Julia set contains an invariant interval on \mathbb{R} , but is not contained in \mathbb{R} .

For $f: z \mapsto z^2 + i$, the Julia set is a “dendrite” (see Figure 3).

For $c \approx 0.12 + 0.74i$, the map $f: z \mapsto z^2 + c$ has an attracting cycle of period 3. Its Julia set is known as the *Douady rabbit* (Figure 4).

No Wandering Domains Theorem and Dynamics on the Fatou Set

A component D of the Fatou set is called *wandering* if $f^n(D) \cap f^m(D) = \emptyset$ for all natural $n > m$.

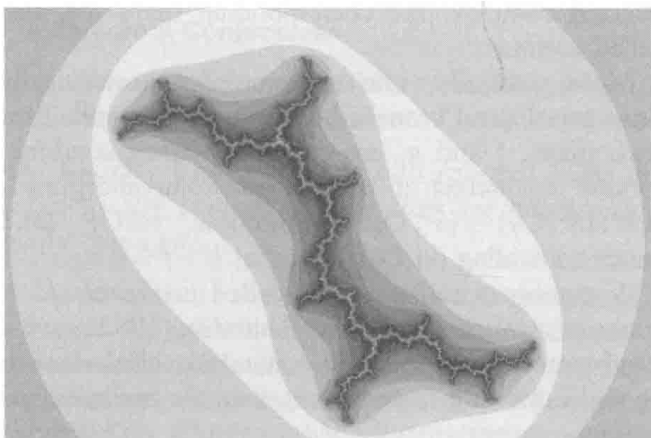


Figure 3 Dendrite.

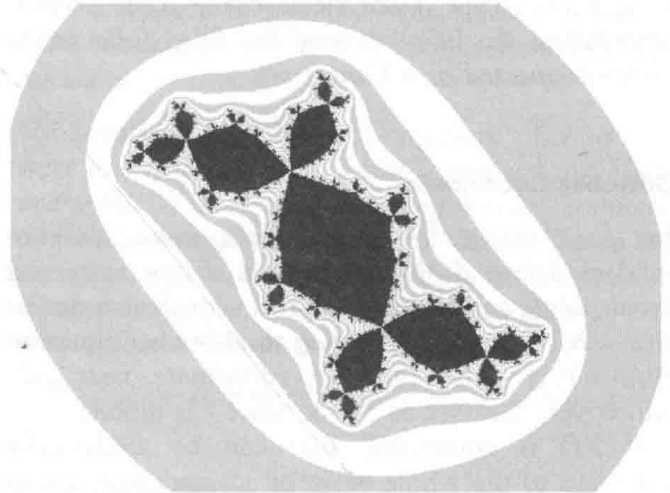


Figure 4 Douady rabbit.

Theorem 3 (Sullivan 1982). *Rational functions do not have wandering domains.*

This theorem is analogous to Ahlfors theorem in the theory of Kleinian groups. Its proof introduced to holomorphic dynamics the methods of *quasiconformal deformations* that has become the basic tool of the subject.

The “no wandering domains theorem” has completed the picture of dynamics on the Fatou set. Namely, for any $z \in F(f)$, one of the following three events may happen:

- z belongs to the basin of attraction of some attracting cycle;
- z belongs to the basin of attraction of some parabolic cycle; and
- for some n , $f^n z$ belongs to a rotation domain.

Here a *rotation domain* is either a Siegel disk, or a *Herman ring*, that is, a topological annulus A such that $f^p(A) = A$ for some $p \in \mathbb{N}$ and $f^p|_A$ is conformally equivalent to an irrational rotation $z \mapsto e^{2\pi i} z$ of a round annulus $\{z: 1 < |z| < R\}$. Note that Herman rings cannot occur for polynomial maps.

More Properties of the Julia Set

There are two more useful characterizations of the Julia set:

- If z is not an attracting periodic point and does not belong to a rotation domain, then the set of accumulation points of the full preimages $f^{-n}z$ is equal to $J(f)$.
- The Julia set is the closure of the set of repelling periodic points.

In the polynomial case, the Julia set $J(f)$ (and the filled Julia set $K(f)$) is connected if and only if the critical points do not escape to ∞ (in other words,

$C_f \subset K(f)$). In the quadratic case, the *Basic Dichotomy* holds: the Julia set (and the filled Julia set) is either connected or a Cantor set.

Böttcher Coordinate

Let $f = z^d + a_1 z^{d-1} + \dots + a_d$ be a monic polynomial of degree $d \geq 2$. Then ∞ is a superattracting fixed point, and hence there is a univalent function $B(z) = B_f(z)$ near ∞ satisfying the Böttcher equation $B(fz) = B(z)^d$ (the *Böttcher coordinate* near ∞). Moreover, $B(z) \sim z$ as $z \rightarrow \infty$ since f is monic.

If $J(f)$ is connected, $B(z)$ can be analytically extended to the whole basin of ∞ , and provides us with the Riemann map $\mathbb{C} \setminus K(f) \rightarrow \mathbb{C} \setminus \bar{\mathbb{D}}$. Otherwise, $B(z)$ extends to a conformal map from some invariant domain Ω_f whose boundary contains a critical point onto $\mathbb{C} \setminus \bar{\mathbb{D}}_R$, where $R = R_f > 1$.

The B -preimage of a straight ray $\{re^{2\pi i\theta} : 0 < r < \infty\}$ is called the *external ray* \mathcal{R}_θ of angle θ . The B -preimage of a round circle $\{re^{2\pi i\theta} : 0 \leq \theta < 1\}$ is called the *equipotential* \mathcal{E}_t of level $t = \log r$. External rays and equipotentials form two orthogonal f -invariant foliations. We let $\mathcal{R}_\theta(t) = \mathcal{R}_\theta \cap \mathcal{E}_t$.

Combinatorial Equivalence

Assume now that $J(f)$ is connected. One says that an external ray \mathcal{R}_θ *lands* at some point $z \in J(f)$ if $\mathcal{R}_\theta(t) \rightarrow z$ as $t \rightarrow 0$. Any external ray of rational angle $\theta = q/p$ with odd p lands at some repelling or parabolic periodic point of period dividing p (Douady and Hubbard 1982). Vice versa, any repelling or parabolic point is a landing point of at least one rational ray as above (Douady 1990s).

Let us consider the following equivalence relation on the set of rational numbers with odd denominators: two such numbers θ and θ' are equivalent if the corresponding rays \mathcal{R}_θ and $\mathcal{R}_{\theta'}$ land at the same point $z \in J(f)$. Two polynomials f and \tilde{f} with connected Julia set are called *combinatorially equivalent* if the corresponding equivalence relations coincide. Notice that topologically equivalent polynomials are combinatorially equivalent.

Parameter Phenomena

Spaces of Rational Functions

Let Rat_d stand for the space of rational functions of degree d . As an open subset of the complex projective space \mathbb{CP}^{2d+1} , it is endowed with the natural topology and complex structure.

Hyperbolic Maps and Fatou's Conjecture

Hyperbolic maps form an important and best-understood class of rational maps (compare with Hyperbolic Dynamical Systems). A rational map f is called *hyperbolic* if one of the following equivalent conditions holds:

- All critical points of f converge to attracting cycles;
- The map is expanding on the Julia set:

$$|Df^n(z)| \geq C\lambda^n, \quad z \in J(f)$$

where $C > 0$, $\lambda > 1$.

For instance, the maps $z \mapsto z^2 + \varepsilon$ for small ε , $z \mapsto z^2 - 1$, and $z \mapsto z^2 + c$ for $c \in \mathbb{R} \setminus [-2, 1/4]$ are hyperbolic. It is easy to see from the first definition that hyperbolicity is a *stable* property, that is, the set of hyperbolic maps is open in the space Rat_d of rational maps of degree d . One of the central open problems in holomorphic dynamics is to prove that this set is also dense. This problem is known as *Fatou's conjecture*.

Postcritically Finite Maps and Thurston's Theory

A rational map is called *postcritically finite* if the orbits of all critical points are finite. In this case, any critical point c is either a superattracting periodic point, or a repelling *preperiodic* point (i.e., $f^n c$ is a repelling periodic point for some n). If all critical points of f are preperiodic, then $J(f) = \hat{\mathbb{C}}$.

Important examples of postcritically finite maps with $J(f) = \hat{\mathbb{C}}$ come from the theory of elliptic functions. Namely, let $\mathcal{P}_\tau : \mathbb{C}/\Gamma_\tau \rightarrow \hat{\mathbb{C}}$ be the Weierstrass \mathcal{P} -function, where Γ_τ is the lattice in \mathbb{C} generated by 1 and τ , $\text{Im } \tau > 0$. It satisfies the functional equation $\mathcal{P}_\tau(nz) = f_{\tau,n}(\mathcal{P}(z))$, where $f_{\tau,n}$ is a rational function. These functions called *Lattés examples* possess the desired properties. (For some special lattices, n can be selected complex: the corresponding maps are also called Lattés.)

More generally, one can consider postcritically finite topological branched coverings $f : S^2 \rightarrow S^2$. Two such maps, f and g , are called *Thurston combinatorially equivalent* if there exist homeomorphisms $h, h' : (S^2, O_f) \rightarrow (S^2, O_g)$ homotopic rel O_f (and hence coinciding on O_f) such that $h' \circ f = h \circ g$.

A combinatorial class is called *realizable* if it contains a rational function. Thurston (1982) gave a combinatorial criterion for a combinatorial class to be realizable. If it is realizable, then the realization is *unique*, except for Lattés examples (*Thurston's Rigidity Theorem*).

Structural Stability and Holomorphic Motions

A map $f \in \text{Rat}_d$ is called *J-stable* if for any maps $g \in \text{Rat}_d$ sufficiently close to f , the maps $f|J(f)$ and $g|J(g)$ are topologically conjugate, and moreover, the conjugacy $h_g: J(f) \rightarrow J(g)$ is close to id. Thus, the Julia set $J(f)$ moves continuously over the set of J-stable maps. The following result proves a weak version of Fatou's conjecture:

Theorem 4 (Lyubich and Mañé-Sad-Sullivan 1983). *The set of J-stable maps is open and dense in Rat_d . Moreover, the set of unstable maps is the closure of maps that have a parabolic periodic point.*

A map $f \in \text{Rat}_d$ is called *structurally stable* if for any maps $g \in \text{Rat}_d$ sufficiently close to f , the maps f and g are topologically conjugate on the whole sphere, and moreover, the conjugacy $h_g: \hat{\mathbb{C}} \rightarrow \hat{\mathbb{C}}$ is close to id. The set of structurally stable maps is also open and dense in Rat_d (Mañé-Sad-Sullivan).

The proofs make use of the theory of holomorphic motions developed for this purpose but having much broader range of applications in dynamics and analysis. Let X be a subset of $\hat{\mathbb{C}}$, and let $h_\lambda: X \rightarrow \hat{\mathbb{C}}$ be a family of injections depending on parameter $\lambda \in \Lambda$ in some complex manifold with a marked point λ_* . Assume that $h_{\lambda_*} = \text{id}$ and that the functions $\lambda \mapsto h_\lambda(z)$ are holomorphic in λ for any $z \in X$. Such a family of injections is called a *holomorphic motion*.

A holomorphic motion of any set X over Λ extends to a holomorphic motion of the whole sphere $\hat{\mathbb{C}}$ over some smaller manifold $\Lambda' \subset \Lambda$ (Bers-Royden, Sullivan-Thurston 1986). If h_λ is a holomorphic motion of an open subset of the sphere, then the maps h_λ are quasiconformal (Mañé-Sad-Sullivan). These statements are usually referred to as the λ -lemma.

If $\Lambda = \mathbb{D}$, then the holomorphic motion of a set $X \subset \hat{\mathbb{C}}$ extends to a holomorphic motion of $\hat{\mathbb{C}}$ over the whole disk \mathbb{D} (Slodkowsky 1991).

Fundamental Conjectures

The above rigidity and stability results led to the following profound conjectures:

QC Rigidity Conjecture *If two rational maps are topologically conjugate, then they are quasiconformally conjugate.*

Let us consider the real projective tangent bundle PT over $\hat{\mathbb{C}}$, with a natural action of the map f . A measurable invariant line field on the Julia set is an invariant measurable section $X \rightarrow \text{PT}$ over an invariant set $X \subset J(f)$ of positive Lebesgue measure. In other words, it is a family of tangent lines $L_z \subset$

$T_z, z \in X$, such that $Df(L_z) = L_{fz}$. Note that such a field can exist only if $J(f)$ has positive Lebesgue measure.

No Invariant Line Fields Conjecture *Let us consider two rational maps, f and \tilde{f} , that are not Lattés examples. If they are quasiconformally conjugate and the conjugacy is conformal on the Fatou set, then they are conjugate by a Möbius transformation. Equivalently, if f is not Lattés, then there are no measurable invariant line fields on $J(f)$.*

This conjecture would imply Fatou's conjecture.

Mandelbrot Set

Let us consider the quadratic family $f_c: z \mapsto z^2 + c$. (Note that any quadratic polynomial is affinely conjugate to a unique map f_c .) The Mandelbrot set classifies parameters c according to the Basic Dichotomy of the subsection "More properties of the Julia set":

$$M = \{c: J(f_c) \text{ is connected}\} = \{c: f_c^n(0) \mapsto \infty\}$$

Note that $\phi_n(c) \equiv f_c^n(0)$ is a polynomial in c of degree 2^{n-1} , and these polynomials satisfy a recursive relation $\phi_{n+1} = \phi_n^2 + c$. Moreover, $M = \{c: |\phi_n(c)| \leq 2, n \in \mathbb{Z}_+\}$, which gives an easy way to make a computer image of M (see Figure 5).

A distinguished curve seen at the picture of M is the *main cardioid* $C = \{c = e^{2\pi i\theta} - e^{4\pi i\theta}/4, \theta \in \mathbb{R}/\mathbb{Z}\}$. For such a $c = c(\theta) \in C$, the map f_c has a neutral fixed point α_c with rotation number θ . For c inside the domain H_0 bounded by C , f_c has an attracting fixed point α_c , and the Julia set $J(f_c)$ is a Jordan curve (see Figure 1).

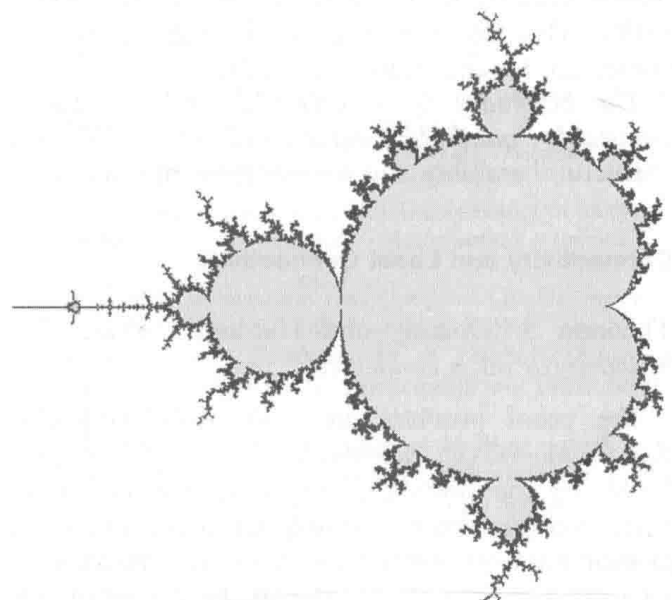


Figure 5 The Mandelbrot set.

At the cusp $c = 1/4 = c(0)$ of the main cardioid, the map f_c has a parabolic point with multiplier 1. This point is also called the *root* of \mathcal{C} . Other parabolic points $c = c(q/p)$ on \mathcal{C} are *bifurcation points*: if one crosses \mathcal{C} transversally at c , then the fixed point α_c “gives birth” to an attracting cycle of period p . This cycle preserves its “attractiveness” within some component $H_{q/p}$ of $\text{int } M$ attached to \mathcal{C} .

On the boundary of $H_{q/p}$, the above attracting cycle becomes neutral, and similar bifurcations happen as one crosses this boundary transversally, etc. In this way we obtain *cascades* of bifurcations and associated necklaces of components of $\text{int } M$. The most famous one is the cascade of *doubling bifurcations* that occur along the real slice of M .

Components of $\text{int } M$ that occur in these bifurcation cascades give examples of hyperbolic components of $\text{int } M$. More generally, a component H of $\text{int } M$ is called *hyperbolic of period p* if the maps $f_c, c \in H$, have an attracting cycle of period p . Many other hyperbolic components become visible if one begins to zoom-in into the Mandelbrot set. Some of them are *satellite*, that is, they are ‘born’ as above by bifurcation from other hyperbolic components. Others are *primitive*. They can be easily distinguished geometrically: primitive components have a cusp at their root, while satellite components are bounded by smooth curves.

Given a hyperbolic component H , let us consider the multiplier $\lambda(c), c \in H$, of the corresponding attracting cycle, as a function of $c \in H$. The function λ univalently maps H onto the unit disk \mathbb{D} (Douady and Hubbard 1982). Thus, there is a single parameter $c_0 \in H$ for which $\lambda(c_0) = 0$, so that f_{c_0} has a *superattracting cycle*. This parameter is called the *center* of H .

Nonhyperbolic components of $\text{int } M$ are called *queer*. Conjecturally, there are no queer components. This conjecture is equivalent to Fatou’s conjecture for the quadratic family.

The boundary of M coincides with the set of *J-unstable quadratic maps* (see the subsection “Structural stability and holomorphic motions”).

Connectivity and Local Connectivity

Theorem 5 (Douady and Hubbard 1982). *The Mandelbrot set is connected.*

The proof provides an explicit uniformization $R_M: \mathbb{C} \setminus M \rightarrow \mathbb{C} \setminus \bar{\mathbb{D}}$. Namely, let $B_c: \Omega_c \rightarrow \mathbb{C} \setminus \mathbb{D}_{R_c}$, $c \in \mathbb{C} \setminus M$, be the Böttcher coordinate near ∞ . Then $R_M(c) = B_c(c)$. This remarkable formula explains the *phase-parameter similarity* between the Mandelbrot set near a parameter $c \in M$ and the corresponding Julia set $J(f_c)$ near the *critical value* c .

The following is the most prominent open problem in holomorphic dynamics:

MLC Conjecture *The Mandelbrot set is locally connected.*

If this is the case, then the inverse map R_M^{-1} extends to the unit circle \mathbb{T} , and the Mandelbrot set can be represented as the quotient of \mathbb{T} modulo certain equivalence relation that can be explicitly described. Thus, we would have an *explicit topological model for the Mandelbrot set* (Douady and Hubbard, Thurston).

The MLC conjecture is equivalent to the following conjecture:

Combinatorial Rigidity Conjecture *If two quadratic maps f_c and $f_{c'}$ with all periodic points repelling are combinatorially equivalent, then $c = c'$.*

In turn, this conjecture would imply, in the quadratic case, the above fundamental conjectures. For a progress towards the MLC conjecture (see *Universality in Mathematical Physics*).

Parabolic Implosion

Parabolic maps $f_{c_0}: z \mapsto z^2 + c_0$ are unstable in a dramatic way. In particular, the Julia set $J(f_c)$ does not depend continuously on c near c_0 . Instead, $J(f_c)$ tends to fill in a good part of $\text{int } J(f_{c_0})$. This phenomenon called *parabolic implosion* has been explored by Douady, Lavaurs, Shishikura, and many others.

Geometric Aspects

Area

One of the basic problems in holomorphic dynamics is *whether a Julia set that does not coincide with $\hat{\mathbb{C}}$ can have positive area*. It would give an example of “observable chaos” that occurs on a topologically small set. It is also related to the No Invariant Line Fields Conjecture.

Maps with strong hyperbolic properties have zero area Julia set. A rational map f is called *Collet–Eckmann* if there exist constants $C > 0$ and $\lambda > 1$ such that:

$$|Df^n(fc)| \geq C\lambda^n, \quad n \in \mathbb{N}$$

for all critical points c . If f is a Collet–Eckmann map with $J(f) \neq \hat{\mathbb{C}}$, then $\text{area } J(f) = 0$ (Przytycki and Rohde 1998) (see *Universality and Renormalization* for more examples). On the other hand, A Douady has set up a compelling program of constructing a Cremer quadratic polynomial $f: z \mapsto e^{2\pi i\theta}z + z^2$ whose Julia set would have *positive area*. Buff and

Cheritat have recently announced that they have completed the program, thus constructing the first example of a Julia set of positive area. (It makes use of a renormalization theorem for parabolic implosion recently announced by Shishikura.)

In the parameter plane, it would be interesting to know *whether the boundary of the Mandelbrot set has zero area.*

Hausdorff Dimension

Hausdorff dimension (HD) gives us a further refinement of fractal sets of zero area. Any Julia set has positive HD. *If f is a polynomial with connected Julia set, then $\text{HD}(J(f)) > 1$ unless f is affinely conjugate to $z \mapsto z^d$ or a Chebyshev polynomial* (Zdunik 1990). If f is a Collet–Eckmann map with $J(f) \neq \hat{\mathbb{C}}$, then $\text{HD } J(f) < 2$ (Przytycki–Rohde 1998). On the other hand, in the quadratic case $f_c: z \mapsto z^2 + c$, $\text{HD}(J(f_c)) = 2$ for a generic parameter $c \in \partial M$. The corresponding parameter result is that $\text{HD}(\partial M) = 2$ (Shishikura 1998). It is based on the parabolic implosion phenomenon.

Conformal Measure

Let $\delta \geq 0$. A Borel measure μ on $\hat{\mathbb{C}}$ is called δ -conformal if

$$\mu(fX) = \int_X |Df|^\delta d\mu$$

for any measurable set X such that $f|_X$ is injective.

Theorem 6 (Sullivan 1983). *Any rational map f has a δ -conformal measure with $\delta \in (0, 2]$ supported on $J(f)$.*

This is a dynamical measure that captures well geometric properties of $J(f)$. For instance, for Collet–Eckmann maps, $\delta = \text{HD}(J(f))$, and μ is equivalent to the Hausdorff measure on $J(f)$ in dimension δ .

The *hyperbolic dimension*, HD_{hyp} of $J(f)$ is the supremum of $\text{HD}(X)$ over all compact invariant hyperbolic subsets of $J(f)$. Denker and Urbanski (1991) proved that $\text{HD}_{\text{hyp}}(J(f))$ is equal to the smallest exponent δ of all δ -conformal measures supported on $J(f)$ (see Universality and Renormalization).

Measure of Maximal Entropy

An f -invariant measure μ is called *balanced* if $\mu(fX) = d\mu(X)$ for any measurable set X such that $f|_X$ is injective (where $d = \deg f$).

Theorem 7 (Brolin 1965, Lyubich 1982). *Any rational map f has a unique balanced measure μ .*

Moreover, preimages of any point z except at most two are equidistributed with respect to μ (meaning that the probability measures $\mu_{n,z}$ that assign mass 1 to every f^n -preimage of z converge weakly to μ as $n \rightarrow \infty$).

For polynomials, the balanced measure coincides with the *harmonic measure* on $J(f)$ (Brolin). (The latter is the charge distribution on the conductor $J(f)$ generated by the unit charge placed at ∞ .) In general, the balanced measure is the *unique measure of maximal entropy* of f , and moreover, *periodic points are equidistributed with respect to μ* (Lyubich).

Measure of maximal entropy is supported on a relatively small measurable set: *its HD is strictly less than $\text{HD}(J(f))$* , unless f is conformally equivalent to $z \mapsto z^d$, a Chebyshev polynomial, or a Lattés example (Zdunik 1990). In the polynomial case, it is supported on a set of HD at most 1 (Manning 1984).

In complex analysis, there has been an extensive study of fractal properties of harmonic measures, providing insights at the balanced measure μ and the other way around (Carleson, Makarov, Jones, Binder, Smirnov, ...)

See also: Fractal Dimensions in Dynamics; Geometric Analysis and General Relativity; Geometric Flows and the Penrose Inequality; Geometric Phases; Polygonal Billiards; Renormalization: General Theory; Renormalization: Statistical Mechanics and Condensed Matter; Universality and Renormalization.

Further Reading

Space limitations prohibit the inclusion of references to all the results quoted in this article. Where an author is quoted in the text, the reader can find the corresponding reference in one of the books listed in this section and in the MatSciNet.

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Holonomic Quantum Fields

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Introduction

The term, holonomic field, was coined by Sato, Miwa, and Jimbo (SMJ) in 1978 and the subject was investigated by them in a series of five long papers and many shorter notes in the period from 1978–81 (Sato *et al.* 1979a, 1979b, 1979c, 1980, Tracy and Widom 1994). The term refers to a special class of two-dimensional interacting quantum field theories whose n point correlations can be expressed in terms of the solution to a holonomic system of differential equations. A holonomic system is an overdetermined system of differential equations with only a finite-dimensional family of solutions. There is a sense in which these interacting systems with infinitely many degrees of freedom have a finite-dimensional substrate (at the level of n point functions for fixed n). After developing their theory, SMJ realized that such quantum fields made an earlier appearance in work of Thirring and Federbush. The models considered by Thirring and Federbush are self-interacting fermionic systems whose nonlinear classical field equations have solutions that are an explicit nonlinear transformation of solutions to the free field equations. This inspired the idea of trying to study these models by “quantizing” the nonlinear transformation. Expressions were obtained for the correlations and S-matrix but the connection with deformation theory was not understood until the SMJ work.

In what follows we will sketch the SMJ theory and discuss some of its offshoots. There is one circumstance that it might help the reader to be aware of even though it will be mostly glossed over. Quantum fields in one space and one time dimension have correlations which transform under the symmetries of spacetime with metric signature (1,1). Since the work of Osterwalder and Schrader, it is customary to pass back and forth between this Minkowski regime and the Schwinger functions obtained by analytically continuing the n point functions to pure imaginary values for the time variable where they possess the rotational symmetries associated with a positive-definite metric. The Ising model, which we take up next, is naturally considered in the Euclidean domain where the correlations have an interpretation in statistical mechanics as the expected value of a product of random variables. Ultimately, the SMJ deformation analysis is done in the Euclidean domain.

The Two-Dimensional Ising Model

The SMJ theory was inspired by, and provides an attractive setting for, an earlier result of Wu, McCoy, Tracy, and Baruch (WMTB), concerning the spin–spin scaling functions of the two-dimensional Ising model (Wu *et al.* 1976). Since the Ising model is the example with the most direct significance for physics, we will take some time to explain the WMTB result and to sketch the way in which it fits into the SMJ theory.

The Ising model is a statistical model of magnetism on a lattice that incorporates ferromagnetic interactions of nearest-neighbor spins. In the 1920s, Ising solved the model for the one-dimensional lattice and showed that there was no phase transition in the infinite volume limit. Interest in the two-dimensional model intensified dramatically following Onsager’s calculation of the specific heat in the infinite volume limit (see Palmer and Tracy (1981) and references within). His formula for the specific heat was the first instance of a thermodynamic quantity in a nearest-neighbor model which exhibits the sort of discontinuity in temperature dependence expected at a phase transition. For many years, the Ising model served as a testbed for the now accepted notion that the infinite volume limit of Gibbsian statistical mechanics provides a suitable setting for the study of phase transitions.

A configuration for the Ising model on a finite subset, Λ , of the integer lattice, \mathbb{Z}^2 , is a map $C: \Lambda \rightarrow \{+1, -1\}$, which assigns to each site on the lattice either an up spin (+1) or a down spin (−1). The energy function of the Ising model, $E_\Lambda(\sigma)$, is defined by

$$E_\Lambda(\sigma) = -J \sum_{\langle i,j \rangle \in \Lambda} \sigma(i)\sigma(j)$$

for $J > 0$ and a spin configuration σ is a sum over pairs of nearest-neighbor sites i, j in Λ (boundary terms require special consideration). This energy function tends to favor spin configurations, σ , in which the nearest-neighbor spins are aligned in the sense that the Boltzmann weight, $e^{-E_\Lambda(\sigma)/kT}$, is larger for such configurations. In the Gibbs ensemble, which is expected to describe systems in equilibrium at temperature T , the configuration σ occurs with a probability proportional to the Boltzmann weight. The factor k which appears is a conversion factor between thermal and kinetic energy called the Boltzmann constant. It is clear from the formula for the Boltzmann weight that small temperatures (near 0) tend to accentuate the difference in

statistical weights assigned to configurations with different energies, and large temperatures tend to wash out the difference in statistical weights associated to configurations with different energies.

Remarkably, there is a sharp critical temperature $0 < T_c < \infty$ so that for $T < T_c$ the propensity for order built into the energy triumphs in the infinite volume limit $\Lambda \uparrow \mathbb{Z}^2$, and for $T > T_c$ the randomness or disorder associated with high temperatures governs the infinite volume behavior. More specifically, if $T < T_c$ and the infinite volume limit is taken with plus spins assigned to the boundary of Λ , the system exhibits a residual magnetism (there is a positive expected value, $\langle \sigma \rangle$, for the spin per site). This infinite volume plus state is the quintessential example of symmetry breaking – the spin flip symmetry possessed by the bulk energy is broken below T_c in the thermodynamic limit. For $T > T_c$, the spin per site is 0 no matter what boundary conditions are imposed on the infinite volume limit.

Pure equilibrium states both above and below T_c exhibit clustering in the thermodynamic limit (uniqueness for the ground state in field theory). This is the tendency of spin variables $\sigma(a)$ and $\sigma(b)$ at sites $a, b \in \mathbb{Z}^2$ to become statistically independent as the distance $|a - b|$ tends to ∞ . In such a pure state the two-point function, which is the expected value of the product of spin variables, $\langle \sigma(a)\sigma(b) \rangle$, will tend to the square $\langle \sigma \rangle^2$ both below ($\langle \sigma \rangle \neq 0$) and above ($\langle \sigma \rangle = 0$) the critical temperature T_c as $|a - b| \rightarrow \infty$. To leading order, this clustering takes place at an exponential rate, $e^{-|a-b|/\xi(T)}$, for a function $\xi(T)$ called the correlation length. The correlation length $\xi(T) \rightarrow \infty$ as $T \rightarrow T_c$. The scaling limit (from below T_c) of the spin–spin correlation is the leading-order correction to the clustering behavior of the correlations when these correlations are examined at the scale of the correlation length. It is the limit

$$\langle \sigma(a)\sigma(b) \rangle = \lim_{T \uparrow T_c} \frac{\langle \sigma(\xi(T)a)\sigma(\xi(T)b) \rangle_T}{\langle \sigma \rangle_T^2}$$

where the correlations on the right-hand side are thermodynamic correlations on the lattice at temperature T . Since $\langle \sigma \rangle_T$ tends to 0 as $T \rightarrow T_c$, the normalization by $\langle \sigma \rangle_T^2$ on the right produces an “infinite wave function renormalization” in the limit.

Equivalently, one may think of this continuum limit being achieved by letting the lattice spacing shrink to 0 as T approaches T_c so that the correlation length stays fixed on the new scale. The scaling limit from above T_c turns out to be different from the scaling limit from below T_c and since $\langle \sigma \rangle_T = 0$ for $T > T_c$, it is defined by a different wave

function renormalization. The resulting asymptotics are expected to capture quite a lot about what is interesting in the behavior of the correlations near the phase transition. In the late 1970s, the scaling behavior in this model was also a prototype for the emerging connection between renormalization group ideas in quantum field theory and statistical mechanics.

Wu *et al.* (1976) showed that the two-point scaling function, $\langle \sigma(0)\sigma(x) \rangle$, is a function of $r = |x|$ and can be written as

$$\langle \sigma(0)\sigma(x) \rangle = \begin{cases} \cosh(\psi/2) \\ \times \exp \frac{1}{4} \int_r^\infty \left(\sinh^2 \psi - \left(\frac{d\psi}{dt} \right)^2 \right) s ds \\ \times (T \uparrow T_c) \\ \sinh(\psi/2) \\ \times \exp \frac{1}{4} \int_r^\infty \left(\sinh^2 \psi - \left(\frac{d\psi}{dt} \right)^2 \right) s ds \\ \times (T \downarrow T_c) \end{cases} \quad [1]$$

where $\psi = \psi(r)$ satisfies the differential equation,

$$\frac{d}{dr} \left(r \frac{d\psi}{dr} \right) = \frac{r}{2} \sinh(2\psi)$$

The substitution $\eta = e^{-\psi}$ transforms this differential equation into a Painlevé equation of the third kind. This was used by McCoy, Tracy, and Wu (see Palmer and Tracy (1981) and references within) to study the short-distance behavior, $r \rightarrow 0$, of the scaling functions – behavior which is far from manifest in the infinite series expansions obtained for the scaling functions.

Deformation Theory

Sato, Miwa, and Jimbo showed that there was a class of quantum field theories that included the scaling limits of the Ising model which have the property that the n -point correlations are “tau functions” for monodromy-preserving deformations of the Dirac equation in two dimensions. The two-dimensional (Euclidean) Dirac operator is

$$\mathcal{D} = \begin{bmatrix} m & -2\partial \\ -2\bar{\partial} & m \end{bmatrix}$$

with

$$\partial = \frac{1}{2} \left(\frac{\partial}{\partial x} - i \frac{\partial}{\partial y} \right), \quad \bar{\partial} = \frac{1}{2} \left(\frac{\partial}{\partial x} + i \frac{\partial}{\partial y} \right)$$

the usual complex derivatives acting on smooth functions on \mathbb{R}^2 . The monodromy-preserving deformations mentioned above are families of (multivalued) solutions $w(x)$ to

$$\mathcal{D}w = 0 \quad [2]$$

which are branched at points $a_j \in \mathbb{R}^2 (j=1, 2, \dots, n)$ and change by a factor $e^{2\pi i \ell_j}$ as x makes a small circuit about a_j . SMJ (1979b) show that the $L^2(\mathbb{R}^2)$ (square-integrable) solutions $w(x)$ of the Dirac equation with this prescribed branching behavior comprise an n -dimensional subspace of $L^2(\mathbb{R}^2)$. The constants $e^{2\pi i \ell_j}$ are called the monodromy of the solutions and the term “deformation” in the description refers to the fact that the monodromy constants do not change as the branch points a_j are varied. SMJ show that it is possible to choose a basis $w_j(x, a) = w_j(x, a_1, \dots, a_n) (j=1, \dots, n)$ so that the vector

$$W(x, a) := [w_1(x, a), w_2(x, a), \dots, w_n(x, a)]$$

becomes a section for a flat (Dirac compatible) connection in the (x, a) variables. That is,

$$d_{x,a} W = \Omega(x, a) W$$

where $d_{x,a}$ is the exterior derivative in the x and a variables and Ω is a matrix-valued 1-form that satisfies the zero curvature condition,

$$d_{x,a} \Omega = \Omega \wedge \Omega$$

They also introduced the notion of a tau function, $\tau(a)$, for such deformations. The logarithmic derivative $d_a \log \tau(a) = \omega$, where ω is a 1-form on $\mathbb{R}^2 \setminus \{a_1, a_2, \dots, a_n\}$ expressed in terms of the matrix elements of Ω . The 1-form ω introduced by SMJ is shown to be closed when Ω satisfies the zero curvature condition above. The scaling limit of the Ising model is related to the situation for monodromy multipliers -1 and when the scaling limits of correlations are identified as suitable τ -functions in this case, the WMTB result emerges when the nonlinear zero curvature condition is identified with a Painlevé equation.

The connection between the deformation theory and quantum field theory is developed in the computationally intensive paper SMJ (1980). Extensive use is made of local operator product expansions, analytic continuation, and formal series expansions that are infinite-dimensional analogs of Wick-type theorems for finite-dimensional spin representations (developed by SMJ (1978)). One can get a feeling for the source of the connection by recalling that in one of the “exact solutions” of the two-dimensional Ising model the spin operators, $\sigma(a)$, are identified as elements of an infinite spin

representation of the orthogonal group and are characterized by their linear action on Fermionic variables (Palmer and Tracy 1981). In the physics literature, the $\sigma(a)$ are referred to as Bogoliubov transformations. In the scaling limit the associated representation space is the home to a free Fermi field $\psi(x)$, an operator-valued solution to the Dirac equation. Of course, $\psi(x)$ has components $\psi_j(x)$ but for simplicity we will suppress such details in the mostly schematic discussion that follows. For coincident second coordinates $x_2 = a_2$ the Fermi field $\psi(x)$ and $\sigma(a)$ satisfy the commutation relation

$$\sigma(a)\psi(x) = -\text{sgn}(x_1 - a_1)\psi(x)\sigma(a) \quad [3]$$

which is a surviving remnant of the linear action of $\sigma(a)$ on lattice fermions. In the transfer matrix formalism, which is natural for statistical mechanics, translation in the “space” variable x_1 is unitary, but translation in the “time” variable, x_2 , is governed by the transfer matrix, the generator of a contractive semigroup. Because of this, the quantities that are well behaved in this formalism are “time-ordered vacuum expectations”; these involve only “positive” powers of the transfer matrix. Let \mathcal{T} denote the “time”-ordering operator; a sequence of operators depending on coordinates in \mathbb{R}^2 is reordered following \mathcal{T} so that the second coordinates appear in increasing order from left to right. Sign changes are incorporated whenever it is necessary to exchange Fermi type operators like $\psi^*(x)$ and $\psi(y)$ to put them in the correct order. In the Euclidean setting (pure imaginary time) it is well known that

$$G(x, y) = \langle \mathcal{T} \psi^*(x) \psi(y) \rangle$$

is a Green function for the Dirac operator \mathcal{D} (the distribution kernel for \mathcal{D}^{-1}).

This observation and [3] suggests that the hybrid vacuum expectation

$$G(x, y; a) = \frac{\langle \mathcal{T} \psi^*(x) \psi(y) \sigma(a_1) \cdots \sigma(a_n) \rangle}{\langle \mathcal{T} \sigma(a_1) \cdots \sigma(a_n) \rangle}$$

should be the Green function for a Dirac operator with a domain containing “functions” branched at the points a_j having “monodromy” -1 there. It is possible to recast the SMJ analysis so that a Dirac operator, $\mathcal{D}(a)$, on a suitable vector bundle with base $\mathbb{R}^2 \setminus \{a_1, \dots, a_n\}$ becomes the central player (see Palmer *et al.* (1994) and references therein). The data for the vector bundle includes the factors $e^{2\pi i \ell_j}$ incorporated in transition functions for the bundle. The τ -function becomes an infinite determinant (or Pfaffian in the Ising case)

$$\tau(a) = \det \mathcal{D}(a) \quad [4]$$

in the Segal–Wilson sense (see Palmer *et al.* (1994) and references therein). The Green function $G(x, y; a)$ has a finite-rank derivative,

$$d_a G(x, y; a) = \sum_j r_j(x, a) s_j(y, a) da_j + u_j(x, a) v_j(y, a) d\bar{a}_j \quad [5]$$

which is the key result in this version of the SMJ analysis (this observation appears in SMJ (1980) but does not have a central role there). The “wave functions” r , s , u , and v are closely related to the L^2 wave functions w_j described above. Equation [5] is both the source of the deformation equations for r , s , u , and v which arise from $d_a^2 G = 0$ coupled with the rotational and translational symmetries of the Green function, and also of the expression for $d_a \log \tau(a)$ in terms of data associated with the deformation theory. A “transfer matrix” calculation of the determinant allows one to make the connection with the scaling limits of lattice fields including the Ising model (see Palmer *et al.* (1994) and references therein).

The short-distance behavior of the two-point function for the Ising model scaling functions has been rigorously calculated by Tracy and later by Tracy and Widom (see Harnad and Its (2002) and references therein). A less detailed analysis of the short-distance behavior of the n point functions that uses the deformation analysis of the correlations in a crucial way can be found in Palmer (2000).

The Riemann–Hilbert Problem

In SMJ (1979b), a “massless” version of holonomic fields is developed. This concerns monodromy-preserving deformations of the Cauchy–Riemann operator $\bar{\partial}$. The techniques used to study this lead back to the Riemann–Hilbert problem – the problem of determining a linear differential equation in the complex plane with rational coefficients and prescribed monodromy at the poles of the coefficients. More specifically, suppose one is given n distinct points $\{a_1, \dots, a_n\}$ in P^1 , the Riemann sphere, and a base point a_0 distinct from the $a_j, j \neq 0$. Let γ_j denote a simple closed curve based at a_0 which winds counterclockwise once around a_j but has winding number 0 for the other points $a_k, k \neq j$. Choose n invertible $p \times p$ matrices M_j which satisfy the single condition $M_1 M_2 \cdots M_n = I$. Then, the homotopy classes of the curves γ_j are the generators for the fundamental group of the punctured sphere $P^1 \setminus \{a_1, \dots, a_n\}$ with base point a_0 and the map which sends $\gamma_j \rightarrow M_j$ determines a representation of the fundamental group. One version of the

Riemann–Hilbert problem is to find $p \times p$ complex matrices A_j for $j=1, \dots, n$ so that the linear differential equation

$$\frac{dY}{dz} = \sum_j \frac{A_j}{z - a_j} Y \quad [6]$$

has monodromy representation given by $\gamma_j \rightarrow M_j$. This means that the fundamental solution $Y(z)$ defined in a neighborhood of $z=a_0$ and normalized so the $Y(a_0)=I$ (the identity) will become the fundamental solution $Y(z)M_j^{-1}$ after analytic continuation around the curve γ_j . This form of the problem does not always have a solution but when it does, it is interesting to consider deformations $a \rightarrow A_j(a)$ that preserve the monodromy multipliers M_j . Such monodromy-preserving deformations were first considered by Schlesinger in 1912 (see Palmer and Tracy (1981) and references therein) and he discovered that the coefficients A_j must satisfy nonlinear differential equations that, for $a_0 = \infty$, can be written as

$$d_a A_j = \sum_{k \neq j} \frac{A_k - A_j}{a_k - a_j} d(a_k - a_j)$$

SMJ introduced τ -functions associated with these deformations and they gave these τ -functions a quantum field theory interpretation as n point functions. Eventually this theory was extended to include the Birkhoff generalization of the Riemann–Hilbert problem, a generalization which incorporates the additional information needed to fix local holomorphic equivalence at higher-order poles (formal asymptotics and Stokes’ multipliers) (Jimbo and Miwa 1981, Sato *et al.* 1978). Roughly speaking, the problem is to reconstruct a global connection with specified singularities from its local holomorphic equivalence data and its global monodromy representation. Thinking of the differential equation [6] as a holomorphic connection proved very helpful in a geometric reworking of the SMJ analysis given by Malgrange (1983a, 1983b) who showed that the zeros of the τ -function occurred at points where a suitably defined Riemann–Hilbert problem fails to have a solution (see also Palmer (1999) references within). The mathematical significance of massless holonomic quantum fields as (quantized) singular elements of a gauge group is apparent from the SMJ work and later work of Miwa but the possibility of interesting physics in these models does not seem to have been much investigated at this time. These quantum fields are also conformal fields; however, a comprehensive integration into the highly developed formalism of conformal field theory on compact Riemann surfaces has not currently been developed

(an analog of [5] should survive on compact Riemann surfaces but the deformation analysis of the correlations is likely limited to symmetric spaces).

Further Developments

This work on massless holonomic fields and the connection with the Riemann–Hilbert problem is doubtless the aspect of holonomic fields with the most “spin offs” in the mathematics and physics literature. These include an analysis of the delta-function gas done by Jimbo, Miwa, Mori, and Sato in 1981, random matrix models first looked at by Jimbo, Miwa, Mori, and Sato and later systematically investigated by Tracy and Widom (1994), the deformations of line bundles on Riemann surfaces that led to KdV in the work of Segal and Wilson (1985), which emerged from work of Sato, Miwa, Jimbo and collaborators, the analysis of Painlevé equations starting with work of McCoy, Tracy and Wu (see Palmer and Tracy (1981) and references within) and more systematically developed by Its and Novokshenov (1986), and the revival of interest in monodromy-preserving deformations (Harnad and Its 2002).

Holonomic fields are related to free fields in a well-understood way and it is natural to study them in situations where free fields make sense. In particular, they are an interesting testbed for the nonperturbative investigation of the influence of geometry (or curvature) on quantum fields. In Palmer *et al.* (1994), the deformation analysis of τ -functions for holonomic fields is carried out for the Poincaré disk. The two-point functions are shown to be expressible in terms of solutions to the family of Painlevé VI equations. A quantum field theory interpretation of these τ -functions is given by Doyon and there are natural analogs of the scaling limit of the Ising model on the Poincaré disk as well. The role of “spacetime” symmetries in the deformation theory suggests that such analysis will be limited to symmetric spaces. In addition to the plane and the Poincaré disk, the cylinder, the sphere, and the torus round out the possibilities in two dimensions. Lisovyy has recently worked out the analysis for the cylinder, which is important for the study of thermodynamic correlations. It should be possible to recast the analysis of the continuum Ising model on the torus (Zuber and Itzykson 1977) in deformation theoretic terms. It does not appear that the holonomic fields associated with the Dirac operator for the constant curvature metric on the 2-sphere have been studied yet.

See also: Deformation Theory; Integrable Systems: Overview; Isomonodromic Deformations; Riemann–Hilbert Problem; Two-Dimensional Ising Model.

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Homeomorphisms and Diffeomorphisms of the Circle

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Introduction

In this article we consider the following question: which homeomorphisms of the circle transport one given class of continuous functions into another? The allowed classes of functions are Banach spaces contained in $C(\mathbb{T})$, the space of continuous functions on the unit circle \mathbb{T} , and will be defined by the properties of the Fourier series of the functions. Next, we will develop the theory of Poincaré–Denjoy which describes some basic geometric properties about diffeomorphisms of the circle such as existence and properties of the rotation number, classifications of possible orbits of diffeomorphisms, and Denjoy counterexample.

A homeomorphism of the circle is regarded here as a change of variables for periodic functions. So, it will be our major concern to describe the changes of variables that do not affect “too much” the behavior of the Fourier series of the functions in the given class.

We say that a function $h: \mathbb{R} \rightarrow \mathbb{R}$ is a homeomorphism of the circle $\mathbb{T} = \{(x, y) \in \mathbb{R}^2 : x^2 + y^2 = 1\}$, if h itself is a homeomorphism such that $h(t + 2\pi) = h(t) \pm 2\pi$ for all $t \in \mathbb{R}$. It is clear that such function h induces a unique homeomorphism $\tilde{h}: \mathbb{T} \rightarrow \mathbb{T}$ that makes the following diagram commutative:

$$\begin{array}{ccc} \mathbb{T} & \xrightarrow{\tilde{h}} & \mathbb{T} \\ e^{it} \downarrow & & \downarrow e^{it} \\ \mathbb{R} & \xrightarrow{h} & \mathbb{R} \end{array} \quad \text{i.e., } \tilde{h}(e^{it}) = e^{ib(t)}$$

In the same way, we identify functions $\tilde{\psi}: \mathbb{T} \rightarrow \mathbb{C}$ with 2π -periodic functions $\psi: \mathbb{R} \rightarrow \mathbb{C}$.

Let $\mathcal{U}(\mathbb{T})$ be the space of all continuous functions on \mathbb{T} that have uniformly convergent Fourier series, and let $\mathcal{A}(\mathbb{T})$ be the space of all continuous functions on \mathbb{T} with absolute convergent Fourier series.

In 1953, Beurling and Helson proved an important result about the homeomorphisms that preserve the space $\mathcal{A}(\mathbb{T})$: they are rotations and symmetries, that is, if $f \circ h \in \mathcal{A}(\mathbb{T})$ for all $f \in \mathcal{A}(\mathbb{T})$, then the homeomorphism h must have the form $h(t) = t + \alpha$ or $h(t) = -t + \alpha$. It is quite obvious that rotations and symmetries preserve $\mathcal{A}(\mathbb{T})$, since the Fourier coefficients of $f \circ h$ and f have the same modulus, but to prove the converse is very hard. So, homeomorphisms that preserve $\mathcal{A}(\mathbb{T})$ are a very restrict class.

A wider class is obtained when we transport $\mathcal{A}(\mathbb{T})$ into $\mathcal{U}(\mathbb{T})$, that is, $f \circ h \in \mathcal{U}(\mathbb{T})$ for all $f \in \mathcal{A}(\mathbb{T})$. The major object of this article is to study such changes of variables.

We say that a homeomorphism of the circle h is of finite type, if there is an integer ν , satisfying $3 \leq \nu < \infty$, such that h is of class C^ν and

$$|h''(t)| + |h^{(3)}(t)| + \cdots + |h^{(\nu)}(t)| \neq 0, \quad \text{for all } t \in \mathbb{R}$$

In the realm of Fourier analysis, the most important and general result about homeomorphisms of the circle is due to R Kaufman, who showed in 1974 that a finite-type homeomorphism h transports $\mathcal{A}(\mathbb{T})$ into $\mathcal{U}(\mathbb{T})$. We shall analyze in detail such seminal result.

Homeomorphism of the Circle of Finite Type

In this section we prove the theorem of R Kaufman mentioned before, which means that it is sufficient for a homeomorphism of the circle h to have a certain amount of curvature in order to transport $\mathcal{A}(\mathbb{T})$ into $\mathcal{U}(\mathbb{T})$. We present a simple proof of this fact, based on a result due to Stein and Wainger.

If $f: \mathbb{T} \rightarrow \mathbb{C}$ is a continuous function and if

$$\hat{f}_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(t) e^{-int} dt, \quad n \in \mathbb{Z}$$

denote the Fourier coefficients of f , then $f \in \mathcal{A}(\mathbb{T})$ if and only if

$$\sum_{n \in \mathbb{Z}} |\hat{f}_n| = \lim_{N \rightarrow \infty} \sum_{n=-N}^N |\hat{f}_n| < \infty$$

Of course, $\mathcal{A}(\mathbb{T})$ is a Banach space with the norm

$$\|f\|_{\mathcal{A}(\mathbb{T})} = \sum_{n \in \mathbb{Z}} |\hat{f}_n|$$

The space $\mathcal{U}(\mathbb{T})$ is defined as the space of all continuous functions $f: \mathbb{T} \rightarrow \mathbb{C}$ such that

$$\sum_{n=-N}^N \hat{f}_n e^{int} \rightarrow f(t), \quad \text{when } N \rightarrow \infty, \quad \text{for all } t \in [-\pi, \pi]$$

uniformly on \mathbb{T} , that is, $\mathcal{U}(\mathbb{T})$ is the space of continuous functions from \mathbb{T} to \mathbb{C} that are the uniform limit of their Fourier partial sums

$$S_N(f, t) = \sum_{n=-N}^N \hat{f}_n e^{int}$$

Hence, under the natural norm given by

$$\|f\|_{\mathcal{U}(\mathbb{T})} = \sup\{|S_N(f, t)| : N \in \mathbb{N} = \{0, 1, \dots\} \text{ and } t \in [-\pi, \pi]\}$$

the space $\mathcal{U}(\mathbb{T})$ is a Banach space.

We shall prove:

Theorem 1 (Kaufman 1974). *Let h be a homeomorphism of the circle of class C^ν , with $\nu \geq 3$. Suppose that*

$$|h''(t)| + |h^{(3)}(t)| + \dots + |h^{(\nu)}(t)| \neq 0, \quad \text{for all } t \in \mathbb{R}$$

Then, h transports $\mathcal{A}(\mathbb{T})$ into $\mathcal{U}(\mathbb{T})$, that is, $f \circ h \in \mathcal{U}(\mathbb{T})$, whenever $f \in \mathcal{A}(\mathbb{T})$.

It follows from the theorem that an analytic homeomorphism of the circle transports $\mathcal{A}(\mathbb{T})$ into $\mathcal{U}(\mathbb{T})$. To see this, suppose that h is not of finite type. Then, for each $n \geq 3$, there exists $t_n \in [-\pi, \pi]$ such that $h^{(j)}(t_n) = 0$ for all $j \in \{2, \dots, n\}$. Since $\{t_n\}$ has a convergent subsequence, there exists $t \in [-\pi, \pi]$ such that $h^{(j)}(t) = 0$ for all $j \geq 2$. This implies that h'' must be a constant function and, therefore, $h(t) = \pm t + \alpha$. Since we know that this kind of homeomorphism preserves $\mathcal{A}(\mathbb{T})$, we are done.

One can ask why to demand $\nu \geq 3$. The answer is easy. Since $h(t + 2\pi) = h(t) \pm 2\pi$ for all $t \in \mathbb{R}$, it follows that $h'(t + 2\pi) = h'(t)$ for all $t \in \mathbb{R}$, that is, h' is a periodic function of period 2π . So, it will always exist a point $t \in (\pi, \pi)$ such that $h''(t) = 0$.

We can also infer from the theorem that a C^∞ homeomorphism of the circle that has no flat point, that is, no point t such that $h^{(j)}(t) = 0$ for all $j \geq 2$, transports $\mathcal{A}(\mathbb{T})$ into $\mathcal{U}(\mathbb{T})$. This is obvious, because the negation of being of finite type implies the existence of a flat point. It is not true, however, that every C^∞ homeomorphism of the circle transports $\mathcal{A}(\mathbb{T})$ into $\mathcal{U}(\mathbb{T})$.

The proof of the theorem is based on the two lemmas that follows. The first lemma was obtained by Stein and Wainger, who proved it in a more general setting in 1965, although that proof was only published five years later. The second lemma was proved by R Kaufman in 1974.

Lemma 2 (Stein and Wainger 1970). *Let $p(t)$ be a real polynomial of degree d . Then*

$$\begin{aligned} \left| \int_{-r}^r e^{ip(t)} \frac{dt}{t} \right| &\leq 6(2^{d+1}) - 2d - 10 \\ &= 2d + 2 \sum_{k=0}^d [3(2^k) - 2] \end{aligned}$$

for all $r > 0$.

Lemma 3 (Kaufman 1974). *Let f be a real function of class C^k on the interval $[-r, r]$, with $k \geq 2$. Suppose that $1 \leq |f^{(k)}(t)| \leq b$ for all $t \in [-r, r]$. Then*

$$\left| \int_{-r}^r e^{if(t)} \frac{dt}{t} \right| \leq C(k, b)$$

where $C(k, b)$ is a constant that depends only on k and b .

We shall see that Lemma 3 can be proved from Lemma 2 in a quite simple way. The proof given by R Kaufman for Lemma 3 does not make use of Lemma 2 at all. Also, it is not difficult to see that Lemma 2 follows from Lemma 3, if we consider $d \geq 2$. So, they are indeed equivalent results.

Before getting into the proof of these two lemmas, let us state a result which is the primary tool in dealing with oscillatory integrals as those in the lemmas.

Lemma 4 (Van der Corput lemma). *Let f be real valued and smooth in $[a, b]$, with $0 < a < b$. Suppose that $|f^{(k)}(t)| \geq \lambda > 0$ for all $t \in [a, b]$. Then*

$$\left| \int_a^b e^{if(t)} \frac{dt}{t} \right| \leq [3(2^k) - 2] \frac{\lambda^{-1/k}}{a}$$

holds if

- (i) $k \geq 2$, and
- (ii) $k = 1$ and $f'(t)$ is monotonic.

Now, let us prove the two lemmas and Theorem 1.

Proof of Lemma 2 The proof is by induction on the degree of the polynomial. Suppose that $p(t)$ is a polynomial of degree 0, that is, $p(t)$ is a constant function. In this case the result is trivial, since the integral is equal to zero.

By induction, assume that the statement is true for polynomials of degree less than or equal to d . Let

$$p(t) = a_{d+1}t^{d+1} + a_d t^d + \dots + a_1 t + a_0, \quad a_{d+1} \neq 0$$

Make the change of variables $t = |a_{d+1}|^{-1/(d+1)} s$. Then we have

$$\int_{-r}^r e^{ip(t)} \frac{dt}{t} = \int_{-\sigma}^{\sigma} e^{i(q(t) \pm t^{d+1})} \frac{dt}{t}$$

where $\sigma = |a_{d+1}|^{1/(d+1)}r$ and $q(t)$ is a polynomial of degree at most equal to d . Suppose $\sigma > 1$. Then

$$\begin{aligned} \left| \int_{-\sigma}^{\sigma} e^{i(q(t) \pm t^{d+1})} \frac{dt}{t} \right| &\leq \left| \int_1^{\sigma} e^{i(q(-t) \pm (-t)^{d+1})} \frac{dt}{t} \right| \\ &\quad + \left| \int_1^{\sigma} e^{i(q(t) \pm t^{d+1})} \frac{dt}{t} \right| \\ &\quad + \left| \int_{-1}^1 e^{i(q(t) \pm t^{d+1})} \frac{dt}{t} \right| \\ &\leq I + II + III \end{aligned}$$

By Van der Corput lemma, $I \leq [3(2^{d+1}) - 2]$ and $II \leq [3(2^{d+1}) - 2]$, so $I + II \leq 6(2^{d+1}) - 4$. Now

$$\begin{aligned} III &\leq \left| \int_{-1}^1 \left[e^{i(q(t) \pm t^{d+1})} - e^{iq(t)} \right] \frac{dt}{t} \right| + \left| \int_{-1}^1 e^{iq(t)} \frac{dt}{t} \right| \\ &\leq \int_{-1}^1 |t|^d dt + 6(2^{d+1}) - 2d - 10 \\ &\leq 2 + 6(2^{d+1}) - 2d - 10 \end{aligned}$$

since the degree of $q(t)$ is at most equal to d . So

$$\begin{aligned} I + II + III &\leq 6(2^{d+1}) - 4 + 2 + 6(2^{d+1}) - 2d - 10 \\ &= 6(2^{d+1}) - 2(d+1) - 10 \end{aligned}$$

On the other hand, if $\sigma \leq 1$, then

$$\begin{aligned} \left| \int_{-\sigma}^{\sigma} e^{i(q(t) \pm t^{d+1})} \frac{dt}{t} \right| &\leq \left| \int_{-\sigma}^{\sigma} \left[e^{i(q(t) \pm t^{d+1})} - e^{iq(t)} \right] \frac{dt}{t} \right| + \left| \int_{-\sigma}^{\sigma} e^{iq(t)} \frac{dt}{t} \right| \\ &\leq 2 + 6(2^{d+1}) - 2d - 10 \\ &\leq 2 + 6(2^{d+1}) - 2d - 10 + 6(2^{d+1}) - 4 \\ &\leq 6(2^{d+1}) - 2(d+1) - 10 \end{aligned}$$

and the proof is completed. \square

Proof of Lemma 3 Assume first that $r > 1$. Then

$$\begin{aligned} \left| \int_{-r}^r e^{if(t)} \frac{dt}{t} \right| &\leq \left| \int_1^r e^{if(-t)} \frac{dt}{t} \right| + \left| \int_1^r e^{if(t)} \frac{dt}{t} \right| + \left| \int_{-1}^1 e^{if(t)} \frac{dt}{t} \right| \\ &= I + II + III \end{aligned}$$

Since $|f^{(k)}(t)| \geq 1$ and $k \geq 2$, then by Van der Corput lemma, $I \leq [3(2^k) - 2]$ and $II \leq [3(2^k) - 2]$. (Note that we have to assume $k \geq 2$ in order to apply Van der Corput lemma, since we know nothing about the monotonicity of $f'(t)$.)

To evaluate III , we proceed as following:

$$\begin{aligned} f(t) &= f(0) + f'(0)t + \cdots + \frac{f^{(k-1)}(0)}{(k-1)!}t^{k-1} + \frac{f^{(k)}(\sigma_t t)}{k!}t^k \\ &= p(t) + f^{(k)}(\sigma_t t) \frac{t^k}{k!} \end{aligned}$$

where the number σ_t depends on t and $0 < \sigma_t < 1$. So

$$\begin{aligned} \left| \int_{-1}^1 e^{if(t)} \frac{dt}{t} \right| &\leq \left| \int_{-1}^1 \left[e^{i(p(t) + f^{(k)}(\sigma_t t) \frac{t^k}{k!})} - e^{ip(t)} \right] \frac{dt}{t} \right| + \left| \int_{-1}^1 e^{ip(t)} \frac{dt}{t} \right| \\ &\leq b \frac{2}{k!} + 6(2^k) - 2(k-1) - 10 \end{aligned}$$

by Lemma 2, since $p(t)$ is a polynomial of degree at most equal to $k-1$.

On the other hand, if $r \leq 1$, it also follows from Lemma 2 that

$$\begin{aligned} \left| \int_{-r}^r e^{if(t)} \frac{dt}{t} \right| &\leq \left| \int_{-r}^r \left[e^{i(p(t) + f^{(k)}(\sigma_t t) \frac{t^k}{k!})} - e^{ip(t)} \right] \frac{dt}{t} \right| + \left| \int_{-r}^r e^{ip(t)} \frac{dt}{t} \right| \\ &\leq b \frac{2}{k!} + 6(2^k) - 2(k-1) - 10 \end{aligned}$$

Hence

$$\left| \int_{-r}^r e^{if(t)} \frac{dt}{t} \right| \leq C(k, b)$$

and we are done. \square

Proof of Theorem 1 Let h be a homeomorphism of the circle satisfying the hypotheses of the theorem.

We claim: there exists $\delta > 0$ such that, for all $x \in [-\pi, \pi]$, there is k depending on x , with $2 \leq k \leq \nu$, such that $|h^{(k)}(t+x)| \geq \delta$ for all t satisfying $|t| \leq \delta$.

The proof of the claim is simple: suppose that there is no such δ . Then, for each $n \in \mathbb{N}$ and each k with $2 \leq k \leq \nu$, there exist $x_n \in [-\pi, \pi]$ and t_{kn} such that $|t_{nk}| \leq 1/n$ and $|h^{(k)}(t_{nk} + x_n)| < 1/n$. Taking a subsequence if necessary, we have $x_n \rightarrow x \in [-\pi, \pi]$. Also, $t_{kn} \rightarrow 0$ when $n \rightarrow \infty$ for all such k . So, $h^{(k)}(t_{kn} + x_n) \rightarrow h^{(k)}(x)$ when $n \rightarrow \infty$. Since $|h^{(k)}(t_{kn} + x_n)| < 1/n$, we conclude that $h^{(k)}(x) = 0$ for all k with $2 \leq k \leq \nu$, thus reaching a contradiction.

Now, let $f \in \mathcal{A}(\mathbb{T})$. So, $\sum_{n=-\infty}^{\infty} |\hat{f}_n| < \infty$, thus implying that

$$f(t) = \sum_{n=-\infty}^{\infty} \hat{f}_n e^{int} = \lim_{N \rightarrow \infty} \sum_{n=-N}^N \hat{f}_n e^{int}$$

Hence

$$f(h(t)) = \sum_{n=-\infty}^{\infty} \hat{f}_n e^{inh(t)} = \lim_{N \rightarrow \infty} \sum_{n=-N}^N \hat{f}_n e^{inh(t)}$$

Put $g_N(t) = \sum_{n=-N}^N \hat{f}_n e^{inh(t)}$. Since g_N is smooth, we have $g_N \in \mathcal{U}(\mathbb{T})$ for all $N \in \mathbb{N}$. If $g(t)$ stands for $f(h(t))$, then $g_N \rightarrow g$ uniformly, since $f \in \mathcal{A}(\mathbb{T})$. Thus, it suffices to prove that $g \in \mathcal{U}(\mathbb{T})$. This happens if and only if $S_m(g, x) = \sum_{k=-m}^m \hat{g}_k e^{ikx}$ converges uniformly to g as $m \rightarrow \infty$, that is, given $\epsilon > 0$, there exists $m_0 \in \mathbb{N}$ such that $|S_m(g, x) - g(x)| < \epsilon$ for all $m > m_0$ and $x \in [-\pi, \pi]$.

We have

$$\begin{aligned} |S_m(g, x) - g(x)| &\leq |g_N(x) - g(x)| + |S_m(g_N, x) - g_N(x)| \\ &\quad + |S_m(g_N, x) - S_m(g, x)| \end{aligned}$$

for all $m, n \in \mathbb{N}$. Since $g_N \rightarrow g$ uniformly and $g_N \in \mathcal{U}(\mathbb{T})$, the last inequality shows that we need to demonstrate that, for each $\epsilon > 0$, there exists $N_0 \in \mathbb{N}$ such that

$$\begin{aligned} |S_m(g_N, x) - S_m(g, x)| &< \epsilon \\ \forall N > N_0, x \in [-\pi, \pi] \quad \text{and} \quad m \in \mathbb{N} \end{aligned}$$

thus proving that $S_m(g_N, x) \rightarrow S_m(g, x)$ uniformly in x and m when $N \rightarrow \infty$.

But, if $K > N \in \mathbb{N}$, we have

$$\begin{aligned} |S_m(g_N, x) - S_m(g_K, x)| &= \left| \frac{1}{2\pi} \int_{-\pi}^{\pi} (g_N(t+x) - g_K(t+x)) D_m(t) dt \right| \\ &= \left| \frac{1}{2\pi} \int_{-\pi}^{\pi} \left(\sum_{n=-N}^N \hat{f}_n e^{inh(t+x)} - \sum_{n=-K}^K \hat{f}_n e^{inh(t+x)} \right) \right. \\ &\quad \left. \times D_m(t) dt \right| \\ &\leq \left| \frac{1}{2\pi} \int_{-\pi}^{\pi} \left(\sum_{K \geq |n| \geq N} \hat{f}_n e^{inh(t+x)} \right) D_m(t) dt \right| \\ &\leq \frac{1}{2\pi} \sum_{K \geq |n| \geq N} |\hat{f}_n| \left| \int_{-\pi}^{\pi} e^{inh(t+x)} D_m(t) dt \right| \end{aligned}$$

where

$$D_m(t) = \sum_{k=-m}^m e^{ikt} = \frac{\sin(m + (1/2))t}{\sin(t/2)}$$

is the Dirichlet kernel.

Hence, we are done if we show that

$$\left| \int_{-\pi}^{\pi} e^{inh(t+x)} D_m(t) dt \right| \leq C \quad [1]$$

where C is a constant that does not depend on m, n , and x .

To prove that the oscillatory integral above is bounded, we make use of Lemma 3. We have that

$$D_m(t) = \frac{2 \sin(mt)}{t} + O(1)$$

on any compact subset of $(-2\pi, 2\pi)$, that is,

$$\begin{aligned} \left| \frac{\sin(m + (1/2))t}{\sin(t/2)} - \frac{2 \sin(mt)}{t} \right| \\ \leq \left| \frac{t \cos(t/2) - 2 \sin(t/2)}{t \sin(t/2)} \right| + 1 \leq C^* \end{aligned}$$

where the constant C^* does not depend on m , on any compact subset of $(-2\pi, 2\pi)$.

In order to prove [1], consider $x \in [-\pi, \pi]$. We have already proved that there exists k (depending on x), with $2 \leq k \leq \nu$, such that $|h^{(k)}(t+x)| \geq \delta > 0$ for all t such that $|t| \leq \delta$. Therefore,

$$\begin{aligned} \left| \int_{-\pi}^{\pi} e^{inh(t+x)} \frac{\sin(mt)}{t} dt \right| &\leq \left| \int_{-\delta}^{\delta} e^{inh(t+x)} \frac{\sin(mt)}{t} dt \right| \\ &\quad + 2 \log\left(\frac{\pi}{\delta}\right) \end{aligned}$$

We can assume that n is a positive integer: if n is negative, we take complex conjugate; and if $n=0$, the integral is trivially bounded, as we see by integration by parts or by Van der Corput lemma. (Indeed, we do not need to worry about $n=0$, since it is necessary to bound the integral only for large n .)

So, assuming that n is a positive integer, we change variables: define $t=rs$, where $r=n^{-1/k}\delta^{-1/k}$. Since $\sin(mt) = (e^{imt} - e^{-imt})/(2i)$, we have

$$\begin{aligned} \left| \int_{-\delta}^{\delta} e^{inh(t+x)} \frac{\sin(mt)}{t} dt \right| &\leq \left| \int_{-\delta}^{\delta} e^{i[nb(t+x)+mt]} \frac{dt}{t} \right| + \left| \int_{-\delta}^{\delta} e^{i[nb(t+x)-mt]} \frac{dt}{t} \right| \\ &= \left| \int_{-\delta/r}^{\delta/r} e^{i[nb(rs+x)+mrs]} \frac{ds}{s} \right| \\ &\quad + \left| \int_{-\delta/r}^{\delta/r} e^{i[nb(rs+x)-mrs]} \frac{ds}{s} \right| \end{aligned}$$

Put $\phi(t) = nb(rt+x) + mrt$ and $\psi(t) = nb(rt+x) - mrt$. We have $\phi^{(k)}(t) = nr^k h^{(k)}(rt+x)$ and $\psi^{(k)}(t) = nr^k h^{(k)}(rt+x)$. But, since $nr^k = 1/\delta$, we conclude that

$$\begin{aligned} |\phi^{(k)}(t)| &= |\psi^{(k)}(t)| \\ &= \frac{1}{\delta} |h^{(k)}(rt+x)| \geq 1, \quad \forall t \in \left[-\frac{\delta}{r}, \frac{\delta}{r}\right] \end{aligned}$$

Also,

$$\begin{aligned} |\phi^{(k)}(t)| &= |\psi^{(k)}(t)| \leq b_k \\ &= \frac{1}{\delta} \max\{|h^{(k)}(s)|: -2\pi \leq s \leq 2\pi\} \end{aligned}$$

for all $t \in [-\delta/r, \delta/r]$. Therefore, by Lemma 3, we get

$$\begin{aligned} \left| \int_{-\delta/r}^{\delta/r} e^{i\phi(t)} \frac{dt}{t} \right| &\leq C(k, b_k) \\ &\leq \max\{C(j, b_j): 2 \leq j \leq \nu\} \end{aligned}$$

and

$$\begin{aligned} \left| \int_{-\delta/r}^{\delta/r} e^{i\psi(t)} \frac{dt}{t} \right| &\leq C(k, b_k) \\ &\leq \max\{C(j, b_j): 2 \leq j \leq \nu\} \end{aligned}$$

This concludes the proof. \square

Diffeomorphisms of the Circle

In this section we study the circle diffeomorphisms. This theory goes back to Poincaré (1885), who studied circle diffeomorphisms to decide when differential equations on the torus have periodic orbits of a specified type. For this he introduced the rotation number as an important dynamical invariant, which later turned out to be very fruitful in the theory of dynamical systems, and proved that a diffeomorphism with an irrational rotation number is combinatorially equivalent to a rotation with the same rotation number.

Denjoy (1932) constructed examples of diffeomorphisms of class C^1 with irrational rotation number having wandering intervals, in opposition to early ideas of Poincaré. It was necessary to assume that a diffeomorphism without periodic points is more smooth, in fact C^2 , to prove that it is topologically conjugate to the rotation.

The Poincaré Rotation Number

Let $\tilde{h}: \mathbb{T} \rightarrow \mathbb{T}$ be an orientation-preserving homeomorphism. Given such a map, there is a (nonunique) map $h: \mathbb{R} \rightarrow \mathbb{R}$, which is called a lift of \tilde{h} , such that $\tilde{h} \circ p = p \circ h$, where $p: \mathbb{R} \rightarrow \mathbb{T}$ is covering map $p(t) = e^{2\pi i t}$.

A lift, h , of \tilde{h} satisfies:

1. h is monotonically increasing, that is, $h(t_1) \leq h(t_2)$ if $t_1 < t_2$.
2. $h(t+1) = h(t) + 1$ for all $t \in \mathbb{R}$, so $(h - \text{id})$ has period 1.
3. If h_1, h_2 are two lifts of \tilde{h} , then there is an integer k such that $h_2(t) = h_1(t) + k$ for all $t \in \mathbb{R}$.

These conditions immediately yield the following: the transformation $h^k := h \circ \dots \circ h$ is monotonically increasing and $h^k(t+r) = h^k(t) + r$, $t \in \mathbb{R}$, $k \in \mathbb{N}$, $r \in \mathbb{Z}$.

The rotation number gives an asymptotic indication (i.e., in the limit) of the average amount of rotation of a point along an orbit. We start by defining, for a lift h of \tilde{h} , the number

$$\rho_0(h, t) = \lim_{k \rightarrow \infty} \frac{h^k(t) - t}{k}$$

This limit exists and does not depend on the choice of the point $t \in \mathbb{R}$; so, we denote it by $\rho_0(h)$. If h_1, h_2 are two lifts of \tilde{h} , then $\rho_0(h_1, t) - \rho_0(h_2, t)$ is an integer, so

$$\rho(\tilde{h}) := \rho_0(h, t) \bmod 1$$

is well defined. The number $\rho(\tilde{h}) \in [0, 1)$ is called the rotation number of \tilde{h} , and depends continuously on \tilde{h} . For detailed proof, see Katok and Hasselblatt (1995) or Robinson (1999).

Theorem 5 *The rotation number $\rho(\tilde{h})$ is rational if and only if \tilde{h} has a periodic point, this is, there exist $z_0 \in S^1$ and $k \in \mathbb{N}$ such that $\tilde{h}^k(z_0) = z_0$.*

Proof Take a lift h of \tilde{h} such that $h(0) \in [0, 1)$. Suppose that $\rho(h) = q/m$.

If h has no fixed point. Then $h(t) - t \in \mathbb{R} \setminus \mathbb{Z}$ for all $t \in \mathbb{R}$, since $h(t) - t \in \mathbb{Z}$ implies that $p(t)$ is a point fixed for \tilde{h} . In particular, $h(t) - t \neq q$ for all $t \in \mathbb{R}$, since $h - \text{id}$ is continuous and periodic, there exist real numbers $a > 0$ such that $h(t) - t < q - a$ for all $t \in \mathbb{R}$. Then

$$\begin{aligned} h^{km}(t) - h^{(k-1)m}(t) &= h^m[h^{(k-1)m}(t)] - [h^{(k-1)m}(t)] \\ &< q - a, \quad \forall k \in \mathbb{N} \\ \Downarrow \\ h^{km}(t) - t &= \{h^m[h^{(k-1)m}(t)] - [h^{(k-1)m}(t)]\} \\ &\quad + \{h^m[h^{(k-2)m}(t)] - [h^{(k-2)m}(t)]\} \\ &\quad + \{h^m[h^{(k-3)m}(t)] - [h^{(k-3)m}(t)]\} + \dots \\ &\quad + \{h^m(t) - t\} < k(q - a) \end{aligned}$$

So

$$\begin{aligned} \frac{q}{m} = \rho(\tilde{h}) &= \lim_{k \rightarrow \infty} \frac{h^{mk}(t) - t}{mk} \\ &\leq \frac{1}{m} \lim_{k \rightarrow \infty} \frac{k(q - a)}{k} = \frac{q - a}{m} \end{aligned}$$

proving the claim by contraposition.

To see the converse, assume that there exists a periodic point $t_0 \in \mathbb{R}$, that is, there are $m, q \in \mathbb{Z}$ such that $h^m(t_0) = t_0 + q$ then

$$h^{km}(t_0) = t_0 + kq$$

$$\Rightarrow \rho(\tilde{h}) = \lim_{k \rightarrow \infty} \frac{h^{km}(t_0) - t_0}{mk} = \frac{q}{m} \quad \square$$

Corollary 6 A homeomorphism $\tilde{h}: \mathbb{T} \rightarrow \mathbb{T}$ does not have periodic points if and only if the rotation number $\rho(\tilde{h})$ is irrational.

Let R_λ be defined on \mathbb{T} by $R_\lambda(e^{2\pi i t}) = e^{2\pi i(t+\lambda)}$. This map is called a rigid rotation of angle λ and it is easy to see that $h_\lambda(t) = t + \lambda$ is lift of R_λ and that $\rho(R_\lambda) = \rho(h_\lambda) = \lambda \bmod 1$.

In this example we can see the connection between the rationality of the rotation number and the existence of a periodic orbit. Assume $\lambda = m/q$ is rational. Then $h_\lambda^q(t) = t + q\lambda = t + m$. Therefore, every point is periodic with period q . Now, assume that λ is irrational. Since $h_\lambda^n(t) = t + n\lambda$ for all n , then R_λ has no periodic points. In this case, show that every point in \mathbb{T} has a dense orbit.

Now, again let $\tilde{h}: \mathbb{T} \rightarrow \mathbb{T}$ be any orientation-preserving homeomorphism.

Lemma 7 If the rotation number of \tilde{h} is rational, then all periodic orbits have the same period.

Proof If $\rho(\tilde{h}) = m/q$ with $m, q \in \mathbb{Z}$ relatively prime, then we need to show that for any periodic point $z_0 = p(t)$ (where $p(t) = e^{2\pi i t}$ is a covering space projection of \mathbb{T}) there is a lift h of \tilde{h} such that $h(0) \in [0, 1)$ for which $h^q(t) = t + m$. If z_0 is periodic point, then $h^r(t) = t + s$ for some $r, s \in \mathbb{Z}$ and

$$\frac{m}{q} = \rho(\tilde{h}) = \lim_{n \rightarrow \infty} \frac{h^n(t) - t}{nr} = \lim_{n \rightarrow \infty} \frac{ns}{nr} = \frac{s}{r}$$

So that $s = km$ and $r = kq$. Then by monotonicity of h , we have that $h^q(t) = t + m$ as claimed. \square

The Poincaré Denjoy Theorem

A homeomorphism of the circle with rational rotation number has all its orbits asymptotic to periodic ones and this, together with Theorem 5, yields a complete classifications of the possible asymptotic behavior when the rotation number is rational. This motivates the study of the asymptotic behavior of orbits of homeomorphisms with irrational rotation number.

The ω -limit set of a point $z_0 \in \mathbb{T}$ with respect to \tilde{h} is the set $\omega(z_0) = \{z \in \mathbb{T}; \tilde{h}^{n_k}(z_0) \rightarrow z \text{ as } n_k \rightarrow \infty, \text{ for same sequence } \{n_k\}_{k=1}^\infty\}$. The α -limit set $\alpha(z_0)$ of an arbitrary point $z_0 \in \mathbb{T}$ is defined similarly (with $n_k \rightarrow -\infty$ instead $n_k \rightarrow +\infty$).

Any orbit of a rotation R_λ with irrational λ is dense in \mathbb{T} , that is, $\omega(z_0) = \alpha(z_0) = \mathbb{T}$ for all $z_0 \in \mathbb{T}$.

Theorem 8 (Poincaré 1885). Let $\tilde{h}: \mathbb{T} \rightarrow \mathbb{T}$ be an orientation-preserving homeomorphism with irrational rotation number. Then the ω -limit set is independent of x and is either \mathbb{T} or perfect and nowhere dense.

The preceding proposition says that maps with irrational rotation number have either all orbits dense or all orbits asymptotic to a Cantor set.

We say that two maps $f, g: \mathbb{T} \rightarrow \mathbb{T}$ are topologically conjugate if there exists a homeomorphism $h: \mathbb{T} \rightarrow \mathbb{T}$ such that $h \circ f = g \circ h$. This implies that $h \circ f^n = g^n \circ h$ for every integer n . Hence, the conjugacy h maps orbits of f into orbits of g . If a monotone map $l: \mathbb{T} \rightarrow \mathbb{T}$ satisfies $l \circ f = g \circ l$ but is not a necessarily homeomorphism, we only have that inverse image of each point is either a point or a closed interval. We say that l is a semiconjugacy between f and g ; this case l maps orbits or pack of orbits of f into orbits of g .

Theorem 9 (Denjoy 1932). Let $\tilde{f}: \mathbb{T} \rightarrow \mathbb{T}$ be an orientation-preserving diffeomorphism of class C^2 , with irrational rotation number ($\rho(\tilde{f}) = \lambda$). Then \tilde{f} is topologically conjugate to the rigid rotation R_λ .

Note that in spite of the hypothesis of \tilde{f} being C^2 , we obtain only a continuous conjugacy. It took almost 50 years until Michael Herman (1979) was able to solve the more difficult problem of obtaining a smooth conjugacy for rotation number satisfying extra arithmetic conditions.

If \tilde{f} is a circle homeomorphism which does not have periodic points, then there exists a semiconjugacy h between \tilde{f} and a rotation R_λ . If h is not a conjugacy, then there exists a point x of the circle whose inverse image by h is an interval J . Since $h \circ \tilde{f} = R_\lambda \circ h$, we have that $h(\tilde{f}^n(J)) = R_\lambda^n(x)$. It follows that the intervals of the family $\{J, \tilde{f}(J), \tilde{f}^2(J), \dots\}$ are pairwise disjoint, and the ω -limit set of J does not reduce to a periodic orbit. We say that J is a wandering interval of the map \tilde{f} . Thus, C^2 -differentiability implies that \tilde{f} does not have a wandering interval. For details of the proof of Theorem 9, see Melo and Strien (1993).

The Denjoy Example

Denjoy also proved the following result, which shows that the hypothesis of class C^2 is essential.

Theorem 10 (Denjoy 1932). For any irrational number $\lambda \in [0, 1)$, there exists a C^1 -circle diffeomorphism f which has a wandering interval, and rotation number equal to λ .

Proof The construction of a diffeomorphism with wandering interval will be done in the following manner. Given an irrational rotation $R_\lambda(e^{2\pi i t}) = e^{2\pi i(t+\lambda)}$, cut the circle \mathbb{T} at all the points of an orbit $\{z_n = R_\lambda^n(e^{2\pi i t_0}); n \in \mathbb{Z}\}$ of R_λ . In each cut insert a segment J_n of length l_n where $\sum_{n=-\infty}^{\infty} l_n = 1$. We obtain in this manner a new circle longer than the first. The open intervals correspond to the gaps of the Cantor set.

In order to construct f formally. Let l_n be a sequence of positive real numbers with $n \in \mathbb{Z}$ satisfying

- (i) $\lim_{n \rightarrow \pm\infty} (l_{n+1}/l_n) = 1$
- (ii) $\sum_{n=-\infty}^{\infty} l_n = 1$
- (iii) $l_n > l_{n+1}$ for $n \geq 0$
- (iv) $l_n < l_{n+1}$ for $n < 0$ and
- (v) $3l_{n+1} - l_n > 0$ for $n \geq 0$

For example

$$l_n = T(|n| + 2)^{-1}(|n| + 3)^{-1}$$

where

$$T^{-1} = \sum_{n=-\infty}^{\infty} (|n| + 2)^{-1}(|n| + 3)^{-1}$$

Let J_n be a closed interval of length l_n . We place these intervals on the circle in the same order as the order of the orbit $R_\lambda^n(0)$. So to place an interval J_n , consider the sum of the lengths of the intervals J_i where $R_\lambda^i(0)$ is between $R_\lambda^n(0)$ and 0. This determines the placement of J_n .

The next step is to define f on the union of the J_n . It is necessary and sufficient for $f'(t) = 1$ on the endpoint in order for the map to have a continuous derivative when it is extended to the closure. Assume $J_n = [a_n, b_n]$, so $l_n = b_n - a_n$. The integral

$$\int_{a_n}^{b_n} (b_n - t)(t - a_n) dt = \frac{l_n^3}{6}$$

so

$$\frac{6(l_{n+1} - l_n)}{l_n^3} \int_{a_n}^{b_n} (b_n - t)(t - a_n) dt = l_{n+1} - l_n$$

Therefore, if we define f for $x \in J_n$ by

$$f(x) = a_{n+1} + \int_{a_n}^x \left[1 + \frac{6(l_{n+1} - l_n)}{l_n^3} (b_n - t)(t - a_n) \right] dt$$

then $f(b_n) = a_{n+1} + l_n + l_{n+1} - l_n = b_{n+1}$. Also, f is differentiable on J_n with

$$f'(x) = 1 + \frac{6(l_{n+1} - l_n)}{l_n^3} (b_n - x)(x - a_n)$$

Thus, $f'(a_n) = 1 = f'(b_n)$. Notice that for $n < 0$, $l_{n+1} - l_n > 0$, that

$$1 \leq f'(x) \leq 1 + \frac{6(l_{n+1} - l_n)}{l_n^3} \left(\frac{l_n}{2}\right)^2 = \frac{3l_{n+1} - l_n}{2l_n}$$

and $(3l_{n+1} - l_n)/(2l_n)$ goes to 1 as $n \rightarrow -\infty$. Similarly for $n \geq 0$ and $x \in J_n$,

$$1 \geq f'(x) \geq \frac{3l_{n+1} - l_n}{2l_n} > 0$$

so $f'(x)$ goes to 1 as $n \rightarrow +\infty$ uniformly for $x \in J_n$. From these facts, it follows that f is uniformly C^1 on the union of the interiors of the J_n and has a C^1 extension to all of \mathbb{T} .

Let $\Lambda = \mathbb{T} \setminus \bigcup_{n \in \mathbb{Z}} \text{int}(J_n)$. This is a Cantor set. The orbit of a point $x \in \Lambda$ is dense in Λ since it is like the orbit of 0 for R_λ . Thus, $\omega(x) = \Lambda$. If $x \in \text{int}(J_n)$, then there is a smaller interval I whose closure is contained in $\text{int}(J_n)$. Since the interval J_n never returns to J_n but wanders among the other J_k , then J_n is a wandering interval. \square

Further Results

In this section we shall state some additional results about homeomorphisms of the circle in the area of Fourier analysis.

The first result is a theorem of Pál (1914) and Bohr (1935): let $f: \mathbb{T} \rightarrow \mathbb{R}$ be a real continuous function; then, there exists a homeomorphism of the circle h such that $f \circ h \in \mathcal{U}(\mathbb{T})$. The best proof of this theorem is due to Salem (1945). In 1978, Kahane and Katznelson showed that the result is still valid for $f: \mathbb{T} \rightarrow \mathbb{C}$ continuous.

A similar question was posed by Lusin: given a continuous function $f: \mathbb{T} \rightarrow \mathbb{R}$, is there a homeomorphism of the circle h such that $f \circ h \in \mathcal{A}(\mathbb{T})$? The problem remained open until 1981, when Olevskii, Kahane, and Katznelson answered negatively the question: there exists a real (or complex) continuous function f on the circle, such that, for all homeomorphism of the circle h , $f \circ h \notin \mathcal{A}(\mathbb{T})$.

It was proved by the author that there are C^∞ homeomorphisms of the circle, not necessarily of finite type, that transport $\mathcal{A}(\mathbb{T})$ into $\mathcal{U}(\mathbb{T})$. It is a very technical work, published in 1998, and it gives a necessary and sufficient condition for a homeomorphism of the circle with a flat point to transport $\mathcal{A}(\mathbb{T})$ into $\mathcal{U}(\mathbb{T})$.

Finally, the Denjoy theorem (Theorem 9) is rather close to being optimal. The example constructed here can be improved by obtaining a circle diffeomorphism whose first derivatives have Hölder exponent arbitrarily close to 1 (see Katok and Hasselblatt (1995)). Recent

work has dealt with the existence of a differentiable conjugacy between a diffeomorphism f with irrational rotation number λ and R_λ . Arnol, Moser, and Herman have obtained results (see Melo and Strien (1993) for a discussion of this results and references).

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See also: Chaos and Attractors; Ergodic Theory; Generic Properties of Dynamical Systems; Random Dynamical Systems; Wavelets: Mathematical Theory.

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Homoclinic Phenomena

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Introduction

Homoclinic orbits (or motions) were first defined by Poincaré in his treatise on the “restricted three-body problem.” (Poincaré 1987) Further advances were made by Birkhoff (Birkhoff 1960) in the 1930s, and, by Smale in the 1960s. Since that time, they have been studied by many people and have been shown to be intimately related to our understanding of nonlinear dynamical systems. There are many systems which possess homoclinic orbits. In one striking example (as discussed in the book of Moser (1973), they can be used to account for the unbounded oscillatory motion discovered by Sitnikov in the three-body problem. They also commonly occur in two-dimensional mappings derived from periodically forced oscillations (e.g., see the book by Guckenheimer and Holmes (1983).

Roughly speaking, a homoclinic orbit is an orbit of a mapping or differential equation which is both forward and backward asymptotic to a periodic orbit which satisfies a certain nondegeneracy condition called “hyperbolicity.” On its own, such an orbit is only of mild interest. However, these orbits induce quite interesting structures among nearby orbits, and this latter fact is responsible for the main importance of homoclinic orbits. In addition, when homoclinic orbits are created in a parametrized system, many interesting and unexpected phenomena arise.

In this article, we first describe the history and basic properties of homoclinic orbits. Next, we consider some simple polynomial diffeomorphisms of the plane (the so-called Hénon family) which exhibit homoclinic orbits. Subsequently, we discuss a general theorem due to Katok which gives sufficient conditions for the existence of such orbits. Finally, we briefly consider issues related to homoclinic bifurcations and some of their consequences.

Homoclinic Orbits in Diffeomorphisms

Consider a discrete dynamical system given by a C^r diffeomorphism $f: M \rightarrow M$ where M is a C^∞ manifold and r is a positive integer. That is, f is bijective and both f and f^{-1} are r -times continuously differentiable. Given a point $x \in M$, set $x_0 = x$. For non-negative integers n we inductively define $x_{n+1} = f(x_n)$ and $x_{-n-1} = f^{-1}(x_{-n})$. We also write $f^n(x) = x_n$ for n in the set \mathbb{Z} of all integers. The “orbit” of x is the set $O(x) = \{f^n(x): n \in \mathbb{Z}\}$.

A “periodic point” p of f is a point such that there is a positive integer $N > 0$ such that $f^N(p) = p$. The least such number $\tau(p)$ is called the “period” of p . If $\tau(p) = 1$, we call p a “fixed point.” The periodic point p with period τ is called “hyperbolic” if all eigenvalues of the derivative $Df^\tau(p)$ at p have absolute value different from 1. For convenience, we refer to the eigenvalues of $Df^\tau(p)$ as eigenvalues associated to p . If p is a hyperbolic periodic point all of whose associated eigenvalues have norm less than one, we call p a “sink” or “attracting periodic point.” The opposite case in which all associated eigenvalues have norm larger than one is called a “source.” A hyperbolic periodic point p which is neither a source nor a sink is called a “saddle” or “hyperbolic saddle.”

Given a saddle p of period τ , we consider the set $W^s(p) = W^s(p, f)$ of points $y \in M$ which are forward asymptotic to p under the iterates $f^{n\tau}$. That is, the points $y \in M$ such that $f^{n\tau}(y) \rightarrow p$ as $n \rightarrow \infty$. This is called the “stable set” of p . Similarly, we consider the “unstable set” of p which we may define as $W^u(p) = W^u(p, f) = W^s(p, f^{-1})$. The stable manifold theorem guarantees that $W^s(p)$ and $W^u(p)$ are injectively immersed submanifolds of M whose dimensions add up to $\dim M$. In these cases, they are called the stable and unstable manifolds of p , respectively. A point $q \in W^s(p) \cap W^u(p) \setminus \{p\}$ is called a “homoclinic point” of p (or of the pair (f, p)). If the submanifolds $W^s(p)$ and $W^u(p)$ meet transversely at q , then q is called a “transverse homoclinic point.” Otherwise, q is called a “homoclinic tangency.”

In the special case when M is a two-dimensional manifold, the stable and unstable manifolds of a saddle periodic point p are injectively immersed curves in M . A transverse homoclinic point q of p is a point of intersection off p where the curves are not tangent to each other. This is depicted in Figure 1 for the case of a saddle fixed point for the map $H(x, y) = (7 - x^2 - y, x)$, a member of the so-called Hénon family, which we will discuss later. The figure was made using the numerical package “Dynamics” which comes with the book by Nusse and Yorke (1998).

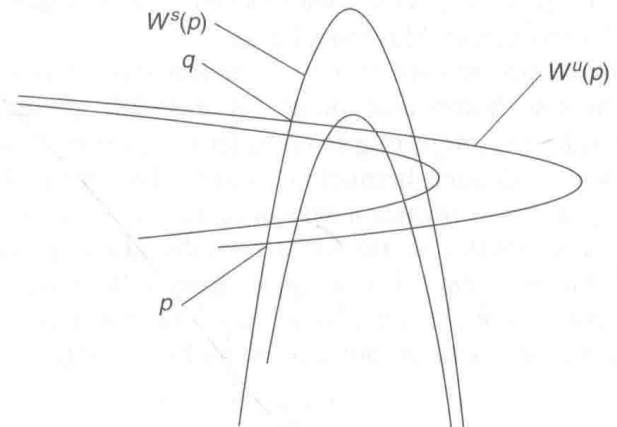


Figure 1 Stable and unstable manifolds in the map $H(x, y) = (7 - x^2 - y, x)$ for the fixed point $p \approx (-3.83, -3.83)$.

One easily sees that every point in the orbit of a transverse homoclinic point q of a hyperbolic saddle fixed point p is again a transverse homoclinic point of p . Also, the curves $W^u(p)$ and $W^s(p)$ are invariant; that is, $f(W^u(p)) = W^u(p)$ and $f(W^s(p)) = W^s(p)$. This implies that the curves $W^u(p)$ and $W^s(p)$ extend, wind around, and accumulate on each other forming a complicated web.

Upon seeing this complicated structure in the restricted three-body problem, Poincaré very poetically wrote (p. 389, Poincaré 1987)

Que l'on cherche à se représenter la figure formée par ces deux courbes et leurs intersections en nombre infini dont chacune correspond à une solution doublement asymptotique, ces intersections forment une sorte de treillis, de tissu, de réseau à mailles infiniment serrées; chacune des deux courbes ne doit jamais se recouper elle-même, mais elle doit se replier sur elle-même d'une manière très complexe pour venir recouper une infinité de fois toutes les mailles du réseau.

On sera frappé de la complexité de cette figure, que je ne cherche même pas à tracer. Rien n'est plus propre à nous donner une idée de la complication du problème des trois corps et en général de tous les problèmes de Dynamique où il n'y a pas d'intégrale uniforme ...

The next major advance concerning homoclinic orbits was made by Birkhoff (1960), who proved that in every neighborhood of a transverse homoclinic point of a surface diffeomorphism, one can find infinitely many distinct periodic points. Birkhoff also presented a symbolic description of the nearby orbits and noticed the analogy with Hadamard's description of geodesics on a surface. Birkhoff's analysis was generalized by Smale to arbitrary dimension, and, in addition, Smale gave a simpler analysis of the associated nearby orbits in terms of compact zero-dimensional

symbolic spaces which we now call “shift spaces” or “topological Markov chains.”

Once one knows that a diffeomorphism f has a transverse homoclinic point for a saddle periodic point p , it is interesting to consider the closure of the orbits of all such homoclinic points. This turns out to be a closed invariant set containing a dense orbit and a countable dense set of periodic saddle points (Newhouse 1980). It is usually called a “homoclinic closure” or h -closure. These sets form the basis of chaotic or irregular motions in nonlinear systems.

The Smale Horseshoe Map and Associated Symbolic System

To understand the geometric picture discovered by Smale, it is best to start with a concrete example of a diffeomorphism of the plane known as the “Smale horseshoe diffeomorphism.”

Given any homeomorphism $f: X \rightarrow X$ on a space X and a subset $U \subset X$, let us define $I(f, U)$ to be the set of points $x \in X$ such that $f^n(x) \in U$ for every integer n . Thus, we have

$$I(f, U) = \bigcap_{n \in \mathbb{Z}} f^n(U)$$

We call $I(f, U)$ the invariant set of f in U , or, alternatively, the invariant set of the pair (f, U) .

We now construct a special diffeomorphism f of the Euclidean plane to itself in which $U = Q$ is the unit square and for which $I(f, U)$ has a very interesting structure. It is this map which is usually known as the Smale horseshoe map.

Let $Q = [0, 1] \times [0, 1]$ be the unit square in the plane \mathbb{R}^2 . Let $0 < \alpha < 1/2$, and consider a diffeomorphism $f: \mathbb{R}^2 \rightarrow \mathbb{R}^2$ which is a composition of two diffeomorphisms $f = T_2 \circ T_1$ as follows. The map $T_1(x, y) = (\alpha^{-1}x, \alpha y)$ contracts vertically, expands horizontally, and maps Q to the thin rectangle $Q_1 = \{(x, y) : 0 \leq x \leq \alpha^{-1}, 0 \leq y \leq \alpha\}$ which is short and wide. The map T_2 bends the right side of Q_1 up and around so that $T_2(Q_1) = f(Q)$ has the shape of a “horseshoe” or “rotated arch.” We arrange for T_2 to take the lower-right corner of Q_1 up to the upper-left corner of Q in such a way that $f(Q)$ meets Q in two full width subrectangles which we call R_1 and R_2 . This can be done in such a way that the preimages $R_1^{-1} = T_1^{-1}(R_1)$ and $R_2^{-1} = T_1^{-1}(T_2^{-1}(R_2))$ are both full-height subrectangles of Q , and the restricted maps $f_1 \stackrel{\text{def}}{=} f|_{R_1^{-1}}$ and $f_2 \stackrel{\text{def}}{=} f|_{R_2^{-1}}$ are both affine. Thus, we arrange that f_1 is simply the restriction of T_1 to R_1^{-1} , and the map f_2 can be expressed in formulas as $f_2(x, y) = (-\alpha^{-1}x + \alpha^{-1}, -\alpha y + 1)$. This construction implies that f will have the origin $p = (0, 0)$ as a

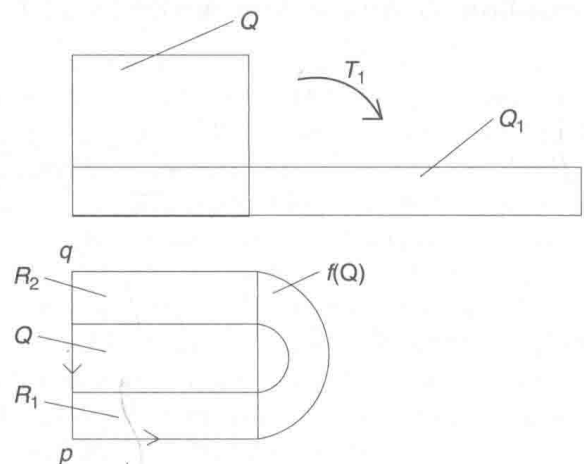


Figure 2 The horseshoe map.

hyperbolic fixed point. We label the upper-left corner $(0, 1)$ of Q with the letter q . It follows that the bottom and left edges of Q will be in the unstable and stable manifolds of p , respectively, and we have indicated this in Figure 2 with small arrows.

The above construction gives us a diffeomorphism f of the plane \mathbb{R}^2 such that $Q_1^+ \stackrel{\text{def}}{=} f(Q) \cap Q = R_1 \cup R_2$ is the union of two full-width subrectangles of Q . We wish to describe $I(f, Q)$. We begin with the sets $Q^+ = \bigcap_{n \geq 0} f^n(Q)$ and $Q^- = \bigcap_{n \leq 0} f^{-n}(Q)$. Thus, Q^+ is simply the set of points in Q whose backward orbits stay in Q , and Q^- is the set of points whose forward orbits stay in Q . For $i = 1, 2$, each rectangle R_i is mapped to a thin horseshoe in $f(Q)$ which meets Q in two full-width subrectangles. Combining these for $i = 1, 2$ gives four full-width rectangles as shaded in Figure 3. Thus, $Q \cap f(Q) \cap f^2(Q)$ consists of these four subrectangles. Figure 3 shows the sets $f^2(Q)$, $f^{-2}(Q)$ as well as the shaded rectangles we just mentioned.

Continuing in this way, one sees that, for each $n > 0$, the set $Q_n^+ = Q \cap f(Q) \cap \dots \cap f^n(Q)$ consists of 2^n full-width subrectangles of Q , each with height

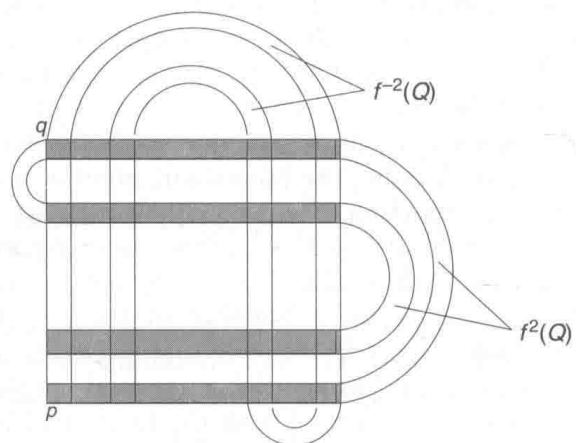


Figure 3 The sets $f^2(Q)$ and $f^{-2}(Q)$ for the horseshoe map f .

α^n . It follows that $Q^+ = \bigcap_n f^n(Q)$ is an interval times a Cantor set. Analogously, Q^- is a Cantor set times an interval, and the set $I(f, Q)$ is a Cantor set in the plane. Let us recall the definition of a Cantor set C in a metric space X . We first define a Cantor space C to be a compact, perfect, totally disconnected metric space. That is, C is a compact metric space, whose connected components are points such that every point x in C is a limit point of $C \setminus \{x\}$. A Cantor set C in a metric space X is a subset which is a Cantor space in the induced subspace (relative) topology.

The dynamics of f on the invariant set $I(f, Q)$ can be conveniently described as follows.

Let $\Sigma_2 = \{1, 2\}^{\mathbb{Z}}$ be the set of doubly infinite sequences of 1's and 2's. Writing elements $a \in \Sigma_2$ as $a = (a_i) = (a_i)_{i \in \mathbb{Z}}$, we define a metric ρ on Σ_2 by

$$\rho(a, b) = \sum_{n \in \mathbb{Z}} \frac{1}{2^{|n|}} |a_i - b_i|$$

The pair (Σ_2, ρ) , then, is a Cantor space.

The “left-shift automorphism” on Σ_2 is the map $\sigma: \Sigma_2 \rightarrow \Sigma_2$ defined by $\sigma(a)_i = a_{i+1}$ for each $i \in \mathbb{Z}$. This is a homeomorphism from Σ_2 to itself. It has a dense orbit and a dense set of periodic points.

For a point $x \in I(f, Q)$, define an element $\phi(x) = a = (a_i) \in \Sigma_2$ by $a_i = j$ if and only if $f^i(x) \in R_j$. It turns out that the map $\phi: I(f, Q) \rightarrow \Sigma_2$ is a homeomorphism such that $\sigma\phi = \phi f$.

In general, given two discrete dynamical systems $f: X \rightarrow X$, and $g: Y \rightarrow Y$, a homeomorphism $h: X \rightarrow Y$ such that $gh = hf$ is called a topological conjugacy from the pair (f, X) to the pair (g, Y) . When such a conjugacy exists, the two systems have virtually the same dynamical properties.

In the present case, one sees that the dynamics of f on $I(f, Q)$ is completely described by that of σ on Σ_2 .

It turns out the the Smale horseshoe map contains essentially all of the geometry necessary to describe the orbit structures near homoclinic orbits. To begin to see this, recall that the left and bottom boundaries of Q were in the stable and unstable manifolds of p . Extending these curves as in Figure 4, one sees that the three corners of Q different from p are, in fact, all transverse homoclinic points of p .

It was a great discovery of Smale that, in the case of a general transverse homoclinic point, one sees the above geometric structure after taking some power f^N of the diffeomorphism f . Thus, we have

Theorem 1 (Smale). *Let $f: M \rightarrow M$ be a C^1 diffeomorphism of a manifold M with a hyperbolic periodic point p and a transverse homoclinic point q of the pair (f, p) . Then, one can find a positive*

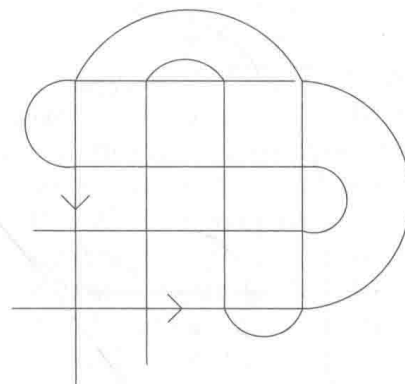


Figure 4 Stable and unstable manifolds in the horseshoe map.

integer N and a compact neighborhood U of the points p and q such that the pair $(f^N, I(f^N, U))$ is topologically conjugate to the full 2-shift (σ, Σ_2) .

In modern language, we can assert that more is true. Let $\Lambda(f) = \bigcup_{0 \leq j < N} f^j(I(f^N, U))$ be the f -orbit of the set $I(f^N, U)$. Then, $\Lambda(f)$ is a compact zero-dimensional hyperbolic basic set for f with $V \stackrel{\text{def}}{=} \bigcup_{0 \leq j < N} f^j(U)$ as an “adapted” or “isolating” neighborhood. This means that $\Lambda(f) = \bigcap_{n \in \mathbb{Z}} f^n(V)$ is a compact, zero-dimensional hyperbolic set (see Robinson (1999) for definitions and related references) contained in the interior of V and $f|_{\Lambda(f)}$ has a dense orbit. If g is C^1 near f , then $\Lambda(g) \stackrel{\text{def}}{=} \bigcap_{n \in \mathbb{Z}} g^n(V)$ is a hyperbolic basic set for g and the pairs $(f, \Lambda(f))$ and $(g, \Lambda(g))$ are topologically conjugate.

To get some appreciation for the magnitude of the contribution here, one might note the complicated arguments employed by Poincaré at the end of Poincaré (1987) to show that so-called heteroclinic points (intersections between stable and unstable manifolds of saddles with different orbits) existed. Birkhoff found a symbolic description (using infinitely many symbols) of the orbits near a transverse homoclinic orbit from which the existence of both infinitely many periodic and heteroclinic points is obvious. Smale extended the treatment of transverse homoclinic points to all dimensions, and found the symbolic description (using two symbols for some iterate of the map) given above. Moreover, Smale proved the “robustness” of these structures: they persist under small C^1 perturbations. Note that Poincaré’s discovery of homoclinic points was in 1899, Birkhoff’s results came in 1935, and Smale’s results came in 1965. Thus, the above advances took over 65 years!

One can understand the geometry of Smale’s construction fairly easily in the two-dimensional case. Let q be the transverse homoclinic point of the saddle fixed point p of the C^r diffeomorphism f on the plane \mathbb{R}^2 . Given a small neighborhood \bar{U} of p , let

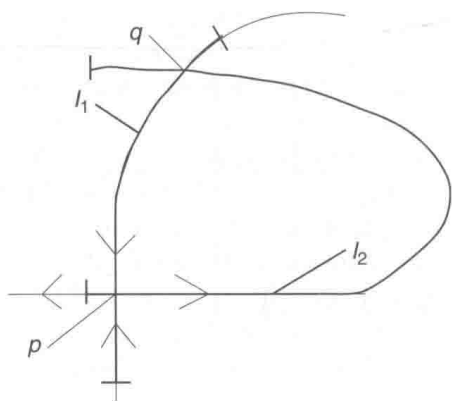


Figure 5 The curves $l_1 \subset W^s(p)$ and $l_2 \subset W^u(p)$.

$W^s(p, \tilde{U})$ denote connected component of $W^s(p) \cap \tilde{U}$ containing p , and define $W^u(p, \tilde{U})$ similarly. We may choose C^r coordinates (x, y) so that in some small neighborhood \tilde{U} of p , the point p corresponds to $(0, 0)$, the set $W^u(p, \tilde{U})$ corresponds to $(y = 0)$, and the set $W^s(p, \tilde{U})$ corresponds to $(x = 0)$. We assume that \tilde{U} is small enough that f in \tilde{U} is closely approximated by its derivative, $Df_{(0,0)}$. Hence, f nearly contracts vertical directions and expands horizontal directions in \tilde{U} .

Take compact arcs $I_1 \subset W^s(p)$ and $I_2 \subset W^u(p)$ both containing the points p and q as in Figure 5.

Let D be a curvilinear rectangle which is a slight thickening of I_1 . The forward iterates $f^i(D)$ will stay near I_1 for a while and then start to approach I_2 . If we choose D appropriately, we can arrange for some high iterate $f^N(D)$ to be a slight thickening of I_2 as in Figure 6. This looks geometrically like the horseshoe map. Let A_1 be the connected component of the intersection $D \cap f^N(D)$ containing p , and let A_2 be the connected component of the intersection $D \cap f^N(D)$ containing q . These sets (which are shaded in Figure 6) play the role of the rectangles R_1 and R_2 , respectively, in the horseshoe construction. We use the set $A_1 \cup A_2$ for U in Theorem 1.

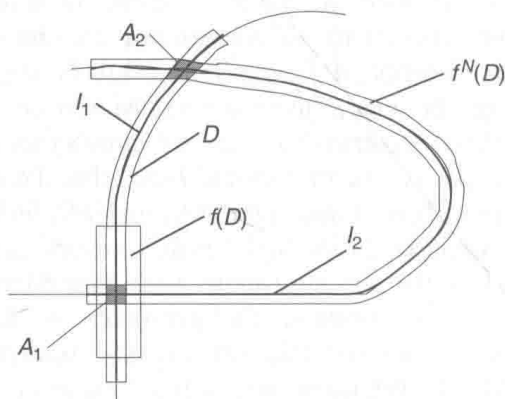


Figure 6 The curvilinear rectangle D and its N th iterate $f^N(D)$ are geometrically like the horseshoe map.

The Hénon Family

To give explicit formulas for the horseshoe map above is somewhat tedious, and it is of interest to note that similar properties occur in maps with simple formulas. Indeed, such properties occur quite often in a well-known family of maps known as the “Hénon family.” As we have mentioned, the map in Figure 1 provides an example.

One may simply define a Hénon map as a diffeomorphism $H = (H_1(x, y), H_2(x, y))$ with inverse $G(x, y) = (G_1(x, y), G_2(x, y))$ such that all the maps $F_i(x, y), G_i(x, y)$ are polynomials of degree at most two. It is known (see, e.g., Friedland and Milnor (1989)) that such maps H have constant Jacobian determinant, and, up to affine conjugacy, may be represented in the form $H = H_{a,b}(x, y) = (a - x^2 - by, x)$ with a, b constants and $b \neq 0$. This makes sense when all the terms are real or complex. In the real case, we speak of the real Hénon family and, in the complex case, we speak of the complex Hénon family.

The real Hénon family was first presented by the physicist M Hénon in 1976 as perhaps the simplest nonlinear diffeomorphism of the plane exhibiting a so-called “strange attractor.” These mappings in the real and complex cases have been the focus of much attention. Our interest here is that, at least for certain parameters a, b , they provide concrete globally defined maps whose dynamics are analogous to that of the horseshoe diffeomorphism. In fact, Devaney and Nitecki (1979) proved (in the real case) that for fixed $b \neq 0$, there is a constant $a_0 > 0$ such that if $a > a_0$, then the set $B_{a,b}$ of bounded orbits of $H_{a,b}$ is a compact zero-dimensional set and the pair $(H_{a,b}, B_{a,b})$ is topologically conjugate to (σ, Σ_2) . In addition, it can be shown that the invariant set $B_{a,b}$ is a single hyperbolic h -closure. Analogous results are true for the complex Hénon family and proofs were originally given in the thesis of Ralph Oberste-Vorth (unpublished) under the supervision of John Hubbard at Cornell University. More recent proofs are in Newhouse (2004) and Hruska (2004). Many interesting results have been obtained for the complex Hénon map by Bedford and Smillie and Sibony and Fornaess (see the references in Hruska (2004)).

Homoclinic Points in Systems with Positive Topological Entropy

There is an invariant of topological conjugacy which is known as the topological entropy. In a certain sense, this gives a quantitative measurement of the amount of complicated or chaotic motion in the system.

Let $f: X \rightarrow X$ be a continuous self-map of the compact metric space (X, d) . For a positive integer $n > 0$, we define an n -orbit to be a finite sequence $O(x, n) = \{x, f(x), \dots, f^{n-1}(x)\}$. Given a positive real number $\epsilon > 0$, we say that two n -orbits $O(x, n)$ and $O(y, n)$ are " ϵ -distinguishable" if there is a $0 \leq j < n$ such that $d(f^j x, f^j y) > \epsilon$. Another way to look at this is the following. Define the so-called d_n -metric on X by setting $d_n(x, y) = \max_{0 \leq j < n} d(f^j x, f^j y)$. Then, the two n -orbits $O(x, n), O(y, n)$ are ϵ -distinguishable if and only if $d_n(x, y) > \epsilon$. It follows from compactness of X and the uniform continuity of each of the maps $f^j, 0 \leq j < n$, that the number $r(n, \epsilon, f)$ of ϵ -distinguishable n -orbits is finite for each given $\epsilon > 0$ and each positive integer n . We define the number

$$h(f) = \lim_{\epsilon \rightarrow 0} \limsup_{n \rightarrow \infty} \frac{1}{n} \log r(n, \epsilon, f)$$

This means that, for some sequence of integers $n_1 < n_2 < \dots$, the map f has roughly $e^{n_i h(f)}$ ϵ -distinguishable n_i -orbits for i large and ϵ small.

The number $h(f)$ is called the topological entropy of the map f . It may be infinite for homeomorphisms, but it is always finite for smooth maps on finite-dimensional manifolds. The number $h(f)$ has many nice properties. For instance, $h(f^N) = Nh(f)$ for every positive integer N , and, if f is a homeomorphism, then $h(f^{-1}) = h(f)$. Further, if f and g are topologically conjugate, then $h(f) = h(g)$. The so-called "variational principle for topological entropy" asserts that $h(f)$ is the supremum of the measure-theoretic entropies of the invariant probability measures for f . Our interest in this invariant here is the following theorem of Katok.

Theorem 2(Katok). *Let f be a C^2 diffeomorphism of a compact two-dimensional manifold M to itself with positive topological entropy. Then, f has transverse homoclinic points.*

In fact, Katok extended this theorem (see the supplement in Hasselblatt and Katok (1995)) to show that, if $h(f) > 0$ and $\epsilon > 0$, then there is a compact zero-dimensional hyperbolic basic set Λ for f such that $h(f, \Lambda) > h(f) - \epsilon$. Thus, one can find nice invariant topologically transitive sets for f (i.e., sets with dense orbits) on which the topological entropies of restriction of f are arbitrarily close to that of f .

This theorem has the interesting consequence that the map $f \rightarrow h(f)$ is lower-semicontinuous on the space of C^2 diffeomorphisms of a surface. It was proved in Newhouse (1989) (and, independently by Yomdin (1987)) that the map $f \rightarrow h(f)$ is upper-semicontinuous on the space of C^∞ diffeomorphisms

of any compact manifold. Combining these results gives the theorem that the map $f \rightarrow h(f)$ is continuous on the space of C^∞ diffeomorphisms on a compact surface, and that positivity of $h(f)$ implies the existence of transverse homoclinic points.

It is also worth noting that, for any continuous self-map $f: M \rightarrow M$ on a compact manifold M , one has the inequality $h(f) \geq \log |\mu|$ where μ is the eigenvalue of largest norm of the induced map f_* on the first real homology group (Manning 1975). Putting this together with Theorem 2 gives the fact that there are whole homotopy classes of diffeomorphisms on surfaces all of whose elements have transverse homoclinic points. For instance, consider a 2×2 matrix

$$L = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

with integer entries, determinant 1, and eigenvalues λ_1, λ_2 with $0 < |\lambda_1| < 1 < |\lambda_2|$. Let $\tilde{L}: T^2 \rightarrow T^2$ be the induced diffeomorphism on the two-dimensional torus T^2 . This is an example of what is called an "Anosov" diffeomorphism. In this case the number μ above is simply λ_2 , and this holds for any diffeomorphism \tilde{f} of T^2 which can be continuously deformed into \tilde{L} . Hence, any such f must have transverse homoclinic points.

Homoclinic Tangencies

Let $\{f_\lambda, \lambda \in [0, 1]\}$ be a parametrized family of C^r diffeomorphisms of the plane with λ an external parameter. It frequently occurs that there is a hyperbolic saddle fixed point p_λ for each parameter λ moving continuously with λ such that, at some value λ_0 , a homoclinic tangency is created at a point q_0 . This means that there are an $\epsilon > 0$, a small neighborhood U of q_0 , and curves $\gamma_\lambda^u \subset W^u(p_\lambda)$, $\gamma_\lambda^s \subset W^s(p_\lambda)$ such that $\gamma_\lambda^u \cap \gamma_\lambda^s = \emptyset$ for $\lambda_0 - \epsilon < \lambda < \lambda_0$, $\gamma_{\lambda_0}^s \cap \gamma_{\lambda_0}^u = \{q_0\}$, and $\gamma_\lambda^u \cap \gamma_\lambda^s$ consists of two distinct points for $\lambda_0 < \lambda < \lambda_0 + \epsilon$. In most cases, the tangency of $\gamma_{\lambda_0}^u$ and $\gamma_{\lambda_0}^s$ at q_0 will be of the second order, and we will assume that occurs here. The geometry is as in Figure 7.

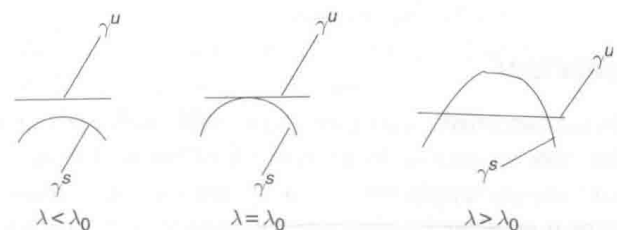


Figure 7 Creation of a homoclinic tangency.

The creation of homoclinic tangencies is part of the general subject of “homoclinic bifurcations.” A recent survey of this subject is in the book by Bonatti *et al.* (2005). Typical results are the following. If $p = p_{\lambda_0}$ is a saddle fixed point whose derivative is area-decreasing (i.e., $|\text{Det}(Df(p))| < 1$), then there are infinitely many parameters λ near λ_0 for which each transverse homoclinic point of p_λ is a limit of periodic sinks (asymptotically stable periodic orbits) (Newhouse 1979, Robinson 1983). In addition, so-called strange attractors and SRB measures appear (Mora and Viana 1993).

Finally, we mention that recently it has been shown that, generically in the C^r topology for $r \geq 2$, homoclinic closures associated to a homoclinic tangency (in dimension 2) have maximal Hausdorff dimension (Theorem 1.6 in Downarowicz and Newhouse (2005)).

See also: Chaos and Attractors; Fractal Dimensions in Dynamics; Generic Properties of Dynamical Systems; Hyperbolic Dynamical Systems; Lyapunov Exponents and Strange Attractors; Saddle Point Problems; Singularity and Bifurcation Theory; Solitons and Other Extended Field Configurations.

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Hopf Algebra Structure of Renormalizable Quantum Field Theory

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Overview

Renormalization theory is a venerable subject put to daily use in many branches of physics. Here, we focus on its applications in quantum field theory, where a standard perturbative approach is provided through an expansion in Feynman diagrams. Whilst

the combinatorics of the Bogoliubov recursion, solved by suitable forest formulas, has been known for a long time, the subject regained interest on the conceptual side with the discovery of an underlying Hopf algebra structure behind these recursions.

Perturbative expansions in quantum field theory are organized in terms of one-particle irreducible (1PI) Feynman graphs. The goal is to calculate the corresponding 1PI Green functions order by order in the coupling constants of the theory, by applying Feynman rules to these 1PI graphs of a

renormalizable theory under consideration. This allows one to disentangle the problem into an algebraic part and an analytic part.

For the algebraic part, one studies Feynman graphs as combinatorial objects which lead to the Lie and Hopf algebras discussed below. Feynman rules then assign analytic expressions to these graphs, with the analytic structure of finite renormalized quantum field theory largely dictated by the underlying algebra.

The objects of interest in quantum field theory are the 1PI Green functions. They are parametrized by the quantum numbers – masses, momenta, spin, and such – of the particles participating in the scattering process under consideration. We call a set of such quantum numbers an external leg structure \underline{r} . For example, the three terms in the Lagrangian of massless quantum electrodynamics correspond to

$$\underline{r} \in \left\{ \text{---}, \text{---}\text{---}, \text{---}\text{---}\text{---} \right\} \quad [1]$$

Note that the Lagrangian L of massless quantum electrodynamics is obtained accordingly as

$$\begin{aligned} L &= \hat{\phi}(\text{---})^{-1} + \hat{\phi}(\text{---}\text{---}) + \hat{\phi}(\text{---}\text{---}\text{---})^{-1} \\ &= \bar{\psi}\partial\psi + \bar{\psi}A\psi + \frac{1}{4}F^2 \end{aligned} \quad [2]$$

where $\hat{\phi}$ are coordinate space Feynman rules.

The renormalized 1PI Green function in momentum space, $G_{\text{R}}^{\underline{r}}(\{g\}; \{p\}, \{m\}; \mu)$, is obtained as the image under renormalized Feynman rules ϕ_{R} applied to a series of graphs:

$$\Gamma^{\underline{r}} = 1 + \sum_{k=1}^{\infty} g^k c_k^{\underline{r}} \equiv 1 + \sum_{\text{res}(\Gamma)=\underline{r}} g^{|\Gamma|} \frac{\Gamma}{\text{Sym}(\Gamma)} \quad [3]$$

Here \underline{r} is a given such external leg structure, while $c_k^{\underline{r}}$ is the finite sum of 1PI graphs having k loops,

$$c_k^{\underline{r}} = \sum_{\substack{\text{res}(\Gamma)=\underline{r} \\ |\Gamma|=k}} \frac{\Gamma}{\text{Sym}(\Gamma)} \quad [4]$$

and $0 < g < 1$ is a coupling constant. The generalization to the case of several couplings $\{g\}$ and masses $\{m\}$ is straightforward. In the above, the sum is over all 1PI graphs with the same given external leg structure. We have denoted the map which assigns \underline{r} to a given graph a residue, for example,

$$\text{res}\left(\text{---}\text{---}\text{---}\right) = \text{---}\text{---}\text{---} \quad [5]$$

The unrenormalized but regularized Feynman rules ϕ assign to a graph a function

$$\begin{aligned} &\phi(\Gamma)(\{g\}; \{p\}, \{m\}; \mu, z) \\ &= \int \prod_{\nu \in \Gamma^{[0]}} \delta^{(4)} \left(\sum_{f \text{ incident } \nu} k_f \right) \prod_{e \in \Gamma^{[1]}} \text{Prop}(k_e) \frac{d^4 k_e}{4\pi^2} \end{aligned} \quad [6]$$

and formally the unrenormalized Green function

$$\begin{aligned} &G_{\text{U}}^{\underline{r}}(\{g\}; \{p\}, \{m\}; \mu, z) \\ &= \phi(\Gamma^{\underline{r}})(\{g\}; \{p\}, \{m\}; \mu, z) \end{aligned} \quad [7]$$

which is a function of a suitably chosen regulator z . Note that in [6] the four-dimensional Dirac- δ distribution guarantees momentum conservation at each vertex and restricts the number of four-dimensional integrations to the number of independent cycles in the graph. It is assumed that the reader is familiar with the readily established fact that these integrals suffer from UV singularities, which render the integration over the momenta in internal cycles ill-defined. We also remind the reader that the problem persists in coordinate space, where one confronts the continuation of products of distributions to regions of coinciding support. We restrict ourselves here to a discussion of the situation in momentum space and refer the reader to the literature for the situation in coordinate space.

Ignoring problems of convergence in the sum over all graphs, the problem of renormalization is to make sense of these functions term by term: We have to determine invertible series $Z^{\underline{r}}(\{g\}, z)$ in the couplings g such that the modified Lagrangian

$$\tilde{L} = \sum_{\underline{r}} Z^{\underline{r}}(\{g\}, z) \hat{\phi}(\underline{r}) \quad [8]$$

produces a perturbation series in graphs that allows for the removal of the regulator z .

This amounts to a transition from unrenormalized to renormalized Feynman rules $\phi \rightarrow \phi_{\text{R}}$. Let us first describe how this transition is achieved using the Lie and Hopf algebra structure of the perturbative expansion, which is described in detail below:

- Decide on the free fields and local interactions of the theory, appropriately specifying quantum numbers (spin, mass, flavor, color, and such) of fields, restricting interactions so as to obtain a renormalizable theory.
- Consider the set of all 1PI graphs with edges corresponding to free-field propagators. Define vertices for local interactions. This allows one to construct a pre-Lie algebra of graph insertions. Antisymmetrize this pre-Lie product to get a Lie algebra \mathcal{L} of graph insertions and define the Hopf algebra \mathcal{H} which is dual to the enveloping algebra $\mathcal{U}(\mathcal{L})$ of this Lie algebra.
- Realize that the coproduct and antipode of this Hopf algebra give rise to the forest formula, which generates local counter-terms upon introducing a Rota-Baxter map, a renormalization scheme in physicists' parlance.

- Use the Hochschild cohomology of this Hopf algebra to show that one can absorb singularities in local counter-terms.
- Determine the corepresentations of this Hopf algebra to identify the sub-Hopf algebras corresponding to time-ordered products in physical fields. This is most easily achieved by rewriting the Dyson–Schwinger equations using Hochschild 1-cocycles.

The last point exhibits close connections, in particular, between the structure of gauge theories and the corepresentation theory of their perturbative Hopf algebras which we discuss below in brief.

This program can be carried out in coordinate space as well as momentum space renormalization. It has given a firm mathematical background to the process of renormalization, justifying the practice of quantum field theory. The notion of locality has achieved a precise formulation in terms of the Hochschild cohomology of the perturbation expansion. In momentum space, this approach emphasizes the connections to number theory, which emerge when one investigates the role of the Hopf algebra primitives, which in turn furnish the Hochschild 1-cocycles underlying locality.

The next sections describe the above setup in some detail.

Lie and Hopf Algebras of Graphs

All algebras are supposed to be over some field \mathbb{K} of characteristic zero, associative and unital, and similarly for coalgebras. The unit (and, by abuse of notation, also the unit map) will be denoted by \mathbb{I} , the counit map by \bar{e} . All algebra homomorphisms are supposed to be unital. A bialgebra $(A = \bigoplus_{i=0}^{\infty} A_i, m, \mathbb{I}, \Delta, \bar{e})$ is called graded connected if $A_i A_j \subset A_{i+j}$ and $\Delta(A_i) \subset \bigoplus_{j+k=i} A_j \otimes A_k$, and if $\Delta(\mathbb{I}) = \mathbb{I} \otimes \mathbb{I}$ and $A_0 = k\mathbb{I}$, $\bar{e}(\mathbb{I}) = 1 \in \mathbb{K}$ and $\bar{e} = 0$ on $\bigoplus_{i=1}^{\infty} A_i$. We call $\ker \bar{e}$ the augmentation ideal of A and denote by P the projection $A \rightarrow \ker \bar{e}$ onto the augmentation ideal, $P = \text{id} - \mathbb{I}\bar{e}$. Furthermore, we use Sweedler's notation, $\Delta(h) = \sum h' \otimes h''$, for the coproduct. We define

$$\text{Aug}^{(k)} = \left(\underbrace{P \otimes \cdots \otimes P}_{k \text{ times}} \right) \Delta^{k-1}, \quad [9]$$

$$A \rightarrow \{\ker \bar{e}\}^{\otimes k}$$

as a map into the k -fold tensor product of the augmentation ideal. We let $A^{(k)} = \ker \text{Aug}^{(k+1)} / \ker \text{Aug}^{(k)}$, $\forall k \geq 1$. All bialgebras considered here are bigraded in the sense that

$$A = \bigoplus_{i=0}^{\infty} A_{(i)} = \bigoplus_{k=0}^{\infty} A^{(k)} \quad [10]$$

where $A_{(k)} \subset \bigoplus_{j=1}^k A^{(j)}$ for all $k \geq 1$. $A_{(0)} \simeq A^{(0)} \simeq \mathbb{K}$.

The first construction we have to study is the pre-Lie algebra structure of 1PI graphs.

The Pre-Lie Structure

For each Feynman graph we have vertices as well as internal and external edges. External edges are edges that have an open end not connected to a vertex. They indicate the particles participating in the scattering amplitude under consideration and each such edge carries the quantum numbers of the corresponding free field. The internal edges and vertices form a graph in their own right. For an internal edge, both ends of the edge are connected to a vertex.

We consider 1PI Feynman graphs. A graph Γ is 1PI if and only if all graphs, obtained by removal of any one of its internal edges, are still connected. Such 1PI graphs are naturally graded by their number of independent loops, the rank of their first homology group $H_{[1]}(\Gamma, \mathbb{Z})$. We write $|\Gamma|$ for this degree of a graph Γ . Note that $|\text{res}(\Gamma)| = 0$, where we let $\text{res}(\Gamma)$ be the graph obtained when all edges in $\Gamma_{\text{int}}^{[1]}$ shrink to a point, as before. Note that the graph obtained in this manner consists of a single vertex, to which the edges $\Gamma_{\text{ext}}^{[1]}$ are attached.

For a 1PI graph Γ , $\Gamma^{[0]}$ denotes its set of vertices and $\Gamma^{[1]} = \Gamma_{\text{int}}^{[1]} \cup \Gamma_{\text{ext}}^{[1]}$ its set of internal and external edges. In addition, let $\omega_{\underline{r}}$ be the number of spacetime derivatives appearing in the corresponding monomial in the Lagrangian.

Having specified free quantum fields and local interaction terms between them, one immediately obtains the set of 1PI graphs. One can then consider for a given external leg structure \underline{r} the set of graphs with that external leg structure. For a renormalizable theory, we can define a superficial degree of divergence,

$$\omega = \sum_{\underline{r} \in \Gamma_{\text{int}}^{[1]} \cup \Gamma^{[0]}} \omega_{\underline{r}} - 4|H_{[1]}(\Gamma, \mathbb{Z})| \quad [11]$$

for each such external leg structure: $\omega(\Gamma) = \omega(\Gamma')$ if $\text{res}(\Gamma) = \text{res}(\Gamma')$; all graphs with the same external leg structure have the same superficial degree of divergence, and only for a finite number of distinct external leg structures \underline{r} will this degree indeed signify a divergence.

This leaves a finite number of external leg structures to be considered to which we restrict ourselves from now. Our first observation is that there is a natural pre-Lie algebra structure on 1PI graphs.

To this end, we define a bilinear operation

$$\Gamma_1 * \Gamma_2 = \sum_{\Gamma} n(\Gamma_1, \Gamma_2; \Gamma) \Gamma \quad [12]$$

where the sum is over all 1PI graphs Γ . Here, $n(\Gamma_1, \Gamma_2; \Gamma)$ is a section coefficient which counts the number of ways in which a subgraph Γ_2 can be reduced to a point in Γ such that Γ_1 is obtained. The above sum is evidently finite as long as Γ_1 and Γ_2 are finite graphs, and the graphs which contribute necessarily fulfill $|\Gamma| = |\Gamma_1| + |\Gamma_2|$ and $\text{res}(\Gamma) = \text{res}(\Gamma_1)$.

One then has the following theorem.

Theorem 1 *The operation $*$ is pre-Lie:*

$$\begin{aligned} & [\Gamma_1 * \Gamma_2] * \Gamma_3 - \Gamma_1 * [\Gamma_2 * \Gamma_3] \\ &= [\Gamma_1 * \Gamma_3] * \Gamma_2 - \Gamma_1 * [\Gamma_3 * \Gamma_2] \end{aligned} \quad [13]$$

which is evident when one rewrites the $*$ -product in suitable gluing operations.

To understand this theorem, note that the equation claims that the lack of associativity in the bilinear operation $*$ is invariant under permutation of the elements indexed 2, 3. This suffices to show that the antisymmetrization of this map fulfills a Jacobi identity. Hence, we get a Lie algebra \mathcal{L} by antisymmetrizing this operation:

$$[\Gamma_1, \Gamma_2] = \Gamma_1 * \Gamma_2 - \Gamma_2 * \Gamma_1 \quad [14]$$

This Lie algebra is graded and of finite dimension in each degree. Let us look at a couple of examples for pre-Lie products:

$$\text{diagram 1} * \text{diagram 2} = \text{diagram 3} + \text{diagram 4} \quad [15]$$

$$\text{diagram 5} * \text{diagram 6} = 2 \cdot \text{diagram 7} \quad [16]$$

$$\text{diagram 8} * \text{diagram 9} = \text{diagram 10} \quad [17]$$

$$\text{diagram 11} * \text{diagram 12} = 2 \cdot \text{diagram 13} \quad [18]$$

$$\text{diagram 14} * \text{diagram 15} = \text{diagram 16} + \text{diagram 17} \quad [19]$$

$$\text{diagram 18} * \text{diagram 19} = \text{diagram 20} \quad [20]$$

Together with \mathcal{L} one is led to consider the dual of its universal enveloping algebra $\mathcal{U}(\mathcal{L})$ using the theorem of Milnor and Moore. For this we use the above grading by the loop number.

This universal enveloping algebra $\mathcal{U}(\mathcal{L})$ is built from the tensor algebra

$$T = \bigoplus_k T^k, \quad T^k = \underbrace{\mathcal{L} \otimes \cdots \otimes \mathcal{L}}_{k \text{ times}} \quad [21]$$

by dividing out the ideal generated by the relations

$$a \otimes b - b \otimes a = [a, b] \in \mathcal{L} \quad [22]$$

Note that in $\mathcal{U}(\mathcal{L})$ we have a natural concatenation product m_* . Furthermore, $\mathcal{U}(\mathcal{L})$ carries a natural Hopf algebra structure with this product. For that, the Lie algebra \mathcal{L} furnishes the primitive elements:

$$\Delta_*(a) = a \otimes 1 + 1 \otimes a, \quad \forall a \in \mathcal{L} \quad [23]$$

It is, by construction, a connected finitely graded Hopf algebra which is co-commutative but not commutative. We can then consider its graded dual, which will be a Hopf algebra $\mathcal{H}(m, \mathbb{I}, \Delta, \bar{e})$ that is commutative but not cocommutative. One finds it upon using a Kronecker pairing

$$\langle Z_\Gamma, \delta_{\Gamma'} \rangle = \begin{cases} 1, & \Gamma = \Gamma' \\ 0, & \text{else} \end{cases} \quad [24]$$

The space of primitives of $\mathcal{U}(\mathcal{L})$ is in one-to-one correspondence with the set $\text{Indec}(\mathcal{H})$ of indecomposables of \mathcal{H} , which is the linear span of its generators. One finds the following theorem.

Theorem 2

$$\langle Z_{\Gamma_1} \otimes Z_{\Gamma_2} - Z_{\Gamma_2} \otimes Z_{\Gamma_1}, \delta_\Gamma \rangle = \langle Z_{[\Gamma_2, \Gamma_1]}, \delta_\Gamma \rangle \quad [25]$$

For example, one finds

$$\begin{aligned} & \left\langle Z_{\text{diagram 21}} \otimes Z_{\text{diagram 22}} - Z_{\text{diagram 22}} \otimes Z_{\text{diagram 21}}, \delta_{\text{diagram 23} + \text{diagram 24}} \right\rangle \\ &= \left\langle Z_{\text{diagram 21}} \otimes Z_{\text{diagram 22}} - Z_{\text{diagram 22}} \otimes Z_{\text{diagram 21}}, \right. \\ & \quad \left. \Delta \left(\delta_{\text{diagram 23} + \text{diagram 24}} \right) \right\rangle \\ &= \left\langle Z_{\text{diagram 25} + \text{diagram 26}} - Z_{\text{diagram 27}}, \delta_{\text{diagram 23} + \text{diagram 24}} \right\rangle \\ &= 2 \end{aligned} \quad [26]$$

\mathcal{H} is a graded commutative Hopf algebra which suffices to describe renormalization theory, as we see in the next section. We have formulated it for the superficially divergent 1PI graphs of the theory with the understanding that the residues of these graphs are in one-to-one correspondence with the terms in the Lagrangian of a given theory. Often, several terms in a Lagrangian correspond to graphs with the same number and type of external legs, but correspond to different form-factor projections of the graph. In such cases, the above approach can be easily adopted considering suitably colored or

labeled graphs. A similar remark applies if one desires to incorporate renormalization of superficially convergent Green functions, which requires nothing more than the consideration of an easily obtained semidirect product of the Lie algebra of superficially divergent graphs with the abelian Lie algebra of superficially convergent graphs.

The Principle of Multiplicative Subtraction

The above algebra structures are available once one has decided on the set of 1PI graphs of interest. We now use them toward the renormalization of any such chosen local quantum field theory.

From the above, 1PI graphs Γ provide the linear generators δ_Γ of the Hopf algebra $\mathcal{H} = \bigoplus_{i=0}^\infty H_i$, where $\mathcal{H}_{\text{lin}} = \text{span}(\delta_\Gamma)$ and their disjoint union provides the commutative product.

Now let Γ be a 1PI graph. We find the Hopf algebra \mathcal{H} as described above to have a coproduct explicitly given as $\Delta: \mathcal{H} \rightarrow \mathcal{H} \otimes \mathcal{H}$:

$$\Delta(\Gamma) = \Gamma \otimes 1 + 1 \otimes \Gamma + \sum_{\gamma \subset \Gamma} \gamma \otimes \Gamma/\gamma \quad [27]$$

where the sum is over all unions of 1PI superficially divergent proper subgraphs, and we extend this definition to products of graphs so that we get a bialgebra.

While the Lie bracket inserted graphs into each other, the coproduct disentangles them. It is this latter operation which is needed in renormalization theory: we have to render each subgraph finite before we can construct a local counter-term. That is precisely what the Hopf algebra structure maps do.

Having a coproduct, two further structure maps of \mathcal{H} are immediate: the counit and the antipode. The counit \bar{e} vanishes on any nontrivial Hopf algebra element, $\bar{e}(1) = 1, \bar{e}(X) = 0$. The antipode is

$$S(\Gamma) = -\Gamma - \sum_{\gamma \subset \Gamma} S(\gamma)\Gamma/\gamma \quad [28]$$

We can work out a few coproducts and antipodes as follows:

$$\text{Aug}^{(2)}(\text{---}\text{---}\text{---}) = 2 \text{---}\text{---}\text{---} \otimes \text{---}\text{---}\text{---} \quad [29]$$

$$\text{Aug}^{(2)}(\text{---}\text{---}\text{---}) = 2 \text{---}\text{---}\text{---} \otimes \text{---}\text{---}\text{---} \quad [30]$$

$$\text{Aug}^{(2)}(\text{---}\text{---}\text{---}) = \text{---}\text{---}\text{---} \otimes \text{---}\text{---}\text{---} \quad [31]$$

$$\text{Aug}^{(2)}(\text{---}\text{---}\text{---}) = 2 \text{---}\text{---}\text{---} \otimes \text{---}\text{---}\text{---} \quad [32]$$

$$\text{Aug}^{(2)}(\text{---}\text{---}\text{---}) = 2 \text{---}\text{---}\text{---} \otimes \text{---}\text{---}\text{---} \quad [33]$$

$$\text{Aug}^{(2)}(\text{---}\text{---}\text{---}) = \text{---}\text{---}\text{---} \otimes \text{---}\text{---}\text{---} \quad [34]$$

We give just one example for an antipode:

$$S(\text{---}\text{---}\text{---}) = -\text{---}\text{---}\text{---} + 2 \text{---}\text{---}\text{---} \quad [35]$$

Note that for each term in the sum $\tilde{\Delta}(\Gamma) = \sum_i \Gamma'_{(i)} \otimes \Gamma''_{(i)}$, we have unique gluing data G_i such that

$$\Gamma = \Gamma''_{(i)} \leftarrow_{G_i} \Gamma'_{(i)}, \quad \forall i \quad [36]$$

These gluing data describe the necessary bijections to glue the components $\Gamma'_{(i)}$ back into $\Gamma''_{(i)}$ so as to obtain Γ : using them, we can reassemble the whole from its parts. Each possible gluing can be interpreted as a composition in the insertion operad of Feynman graphs.

We have by now obtained a Hopf algebra generated by combinatorial elements, 1PI Feynman graphs. Its existence is automatic from the above choices of interactions and free fields. What remains to be done is a structural analysis of these algebras for the renormalizable theories we are confronted with in four spacetime dimensions.

The assertion underlying perturbation theory is the fact that meaningful approximations to physical observable quantities can be found by evaluating these graphs using Feynman rules.

First, as disjoint scattering processes give rise to independent amplitudes, one is led to the study of characters of the Hopf algebra, maps $\phi: \mathcal{H} \rightarrow V$ such that $\phi \circ m = m_V(\phi \otimes \phi)$.

Such maps assign to any element in the Hopf algebra an element in a suitable target space V . The study of tree-level amplitudes in lowest-order perturbation theory justifies assigning to each edge a propagator and to each elementary scattering process a vertex, which define the Feynman rules $\phi(\text{res}(\Gamma))$ and the underlying Lagrangian, on the level of residues of these very graphs. Graphs are constructed from edges and vertices which are provided precisely by the residues of those divergent graphs, hence one is led to assign to each Feynman graph an evaluation in terms of an integral over the continuous quantum numbers assigned to edges or vertices, which leads to the familiar integrals over momenta in closed loops mentioned before.

Then, with the Feynman rules providing a canonical character ϕ , we will have to make one further choice: a renormalization scheme. The need for such a choice is no surprise: after all we are eliminating short-distance singularities in the graphs,

which renders their remaining finite part ambiguous, albeit in a most interesting manner.

Hence, we choose a map $R: V \rightarrow V$, from which we obviously demand that it does not modify the UV-singular structure, and furthermore that it obeys

$$R(xy) + R(x)R(y) = R(R(x)y) + R(xR(y)) \quad [37]$$

which guarantees the multiplicativity of renormalization and is at the heart of the Birkhoff decomposition, which emerges below: it tells us that elements in V split into two parallel subalgebras given by the image and kernel of R . Algebras for which such a map exists are known as Rota–Baxter algebras. The role Rota–Baxter algebras play for associative algebras is similar to the role Yang–Baxter algebras play for Lie algebras. The structure of these algebras allows one to connect renormalization theory to integrable systems. In addition, most of the results obtained initially for a specific renormalization scheme, such as minimal subtraction, can also be obtained, in general, upon a structural analysis of the corresponding Rota–Baxter algebras.

To see how all the above comes together in renormalization theory, we define a further character S_R^ϕ that deforms $\phi \circ S$ slightly and delivers the counter-term for Γ in the renormalization scheme R :

$$\begin{aligned} S_R^\phi(\Gamma) &= -Rm_V(S_R^\phi \otimes \phi \circ P)\Delta \\ &= -R[\phi(\Gamma)] - R\left[\sum_{\gamma \subset \Gamma} S_R^\phi(\gamma)\phi(\Gamma/\gamma)\right] \end{aligned} \quad [38]$$

which should be compared with the undeformed

$$\begin{aligned} \phi \circ S &= m_V(S \circ \phi \otimes \phi \circ P)\Delta \\ &= -\phi(\Gamma) - \sum_{\gamma \subset \Gamma} \phi \circ S(\gamma)\phi(\Gamma/\gamma) \end{aligned} \quad [39]$$

The fact that R is a Rota–Baxter map ensures that S_R^ϕ is an element of the character group \mathcal{G} of the Hopf algebra, $S_R^\phi \in \text{Spec}(\mathcal{G})$. Note that we have now determined the modified Lagrangian:

$$Z^r = S_R^\phi(\Gamma^r) \quad [40]$$

The classical results of renormalization theory follow immediately using this group structure: we obtain the renormalization of Γ by the application of a renormalized character

$$S_R^\phi \star \phi(\Gamma) = m_V(S_R^\phi \otimes \phi)\Delta \quad [41]$$

and Bogoliubov's \bar{R} operation as

$$\begin{aligned} \bar{R}(\Gamma) &= m_V(S_R^\phi \otimes \phi)(\text{id} \otimes P)\Delta(\Gamma) \\ &= \phi(\Gamma) + \sum_{\gamma \subset \Gamma} S_R^\phi(\gamma)\phi(\Gamma/\gamma) \end{aligned} \quad [42]$$

so that

$$S_R^\phi \star \phi(\Gamma) = \bar{R}(\Gamma) + S_R^\phi(\Gamma) \quad [43]$$

Here, $S_R^\phi \star \phi$ is an element in the group of characters of the Hopf algebra, with the group law given by the convolution

$$\phi_1 \star \phi_2 = m_V \circ (\phi_1 \otimes \phi_2) \circ \Delta \quad [44]$$

so that the coproduct, counit, and coinverse (the antipode) give the product, unit, and inverse of this group, as befits a Hopf algebra. This Lie group has the previous Lie algebra \mathcal{L} of graph insertions as its Lie algebra: \mathcal{L} exponentiates to \mathcal{G} .

What we have achieved above is a local renormalization of quantum field theory. Let M^r be a monomial in the Lagrangian L of degree ω_r :

$$M^r = D_r\{\phi\} \quad [45]$$

Then one can prove, using the Hochschild cohomology of \mathcal{H} :

Theorem 3 (*Locality*)

$$Z^r D_r\{\phi\} = D_r Z^r\{\phi\} \quad [46]$$

that is, renormalization commutes with infinitesimal spacetime variations of the fields.

We can now work out the renormalization of a Feynman graph Γ :

$$\begin{aligned} \Delta(\text{diagram}) &= \text{diagram} \otimes \mathbb{I} + \mathbb{I} \otimes \text{diagram} \\ &\quad + 2 \text{diagram} \otimes \text{diagram} \end{aligned} \quad [47]$$

$$\bar{\phi}(\text{diagram}) = \phi(\text{diagram}) + 2S_R^\phi(\text{diagram})\phi(\text{diagram}) \quad [48]$$

$$= \phi(\text{diagram}) - 2R\left[\phi(\text{diagram})\right]\phi(\text{diagram}) \quad [49]$$

$$S_R^\phi(\text{diagram}) = -R[\bar{\phi}(\text{diagram})] \quad [50]$$

$$\begin{aligned} \phi_R(\text{diagram}) &\equiv S_R^\phi \star \phi(\text{diagram}) \\ &= [\text{id} - R] \circ [\bar{\phi}(\text{diagram})] \end{aligned} \quad [51]$$

The formulas [47]–[51] are given in their recursive form. Zimmermann's original forest formula solving this recursion is obtained when we trace our considerations back to the fact that the coproduct can be written in nonrecursive form as a sum over forests, and similarly for the antipode.

Diffeomorphisms of Physical Parameters

In the above, we have effectively obtained a Birkhoff decomposition of the Feynman rules $\phi \in \text{Spec}(\mathcal{G})$ into two characters – $\phi^R_+ = S^\phi_R \star \phi \in \text{Spec}(\mathcal{G})$ and $\phi^R_- = S^\phi_R \in \text{Spec}(\mathcal{G})$ – for any Rota–Baxter map R . Thanks to Atkinson’s theorem, this is possible for any renormalization scheme R . For the minimal subtraction scheme, it amounts to the decomposition of the Laurent series $\phi(\Gamma)(\epsilon)$, which has poles of finite order in the regulator ϵ , into a part holomorphic at the origin and a part holomorphic at complex infinity. This has a particularly nice geometric interpretation upon considering the Birkhoff decomposition of a loop around the origin, providing the clutching data for the two half-spheres defined by that very loop.

Whilst in this manner a satisfying understanding of perturbative renormalization is obtained, the character group \mathcal{G} remains rather poorly understood. On the other hand, renormalization can be captured by the study of diffeomorphisms of physical parameters as, by definition, the range of allowed modification in renormalization theory is determined by the variation of the coefficients of monomials $\hat{\phi}(r)$ of the underlying Lagrangian

$$L = \sum_r Z^r \hat{\phi}(r) \tag{52}$$

Thus, one desires to obtain the whole Birkhoff decomposition at the level of diffeomorphisms of the coupling constants.

The crucial step toward that goal is to realize the role of a standard quantum field-theoretic formula of the form

$$g_{\text{new}} = g_{\text{old}} Z^g \tag{53}$$

where

$$Z^g = \frac{Z^v}{\prod_{e \in \text{res}(v)_{\text{ext}}} \sqrt{Z^e}} \tag{54}$$

for some vertex v , which obtains the new coupling in terms of a diffeomorphism of the old. This formula provides, indeed, a Hopf algebra homomorphism from the Hopf algebra of diffeomorphisms to the Hopf algebra of Feynman graphs, regarding Z^g (a series over counter-terms for all 1PI graphs with the external leg structure corresponding to the coupling g), in two different ways: it is, at the same time, a formal diffeomorphism in the coupling constant g_{old} and a formal series in Feynman graphs. As a consequence, there are two competing coproducts acting on Z_g . That both give the same result defines the required homomorphism,

which transposes to a homomorphism from the largely unknown group of characters of \mathcal{H} to the one-dimensional diffeomorphisms of this coupling.

In summary, one finds that a couple of basic facts enable one to make a transition from the abstract group of characters of a Hopf algebra of Feynman graphs (which, incidentally, equals the Lie group assigned to the Lie algebra with universal enveloping algebra the dual of this Hopf algebra) to the rather concrete group of diffeomorphisms of physical observables. These steps are given as follows:

- Recognize that Z factors are given as counter-terms over a formal series of graphs starting with 1, graded by powers of the coupling, hence invertible.
- Recognize the series Z_g as a formal diffeomorphism, with Hopf algebra coefficients.
- Establish that the two competing Hopf algebra structures of diffeomorphisms and graphs are consistent in the sense of a Hopf algebra homomorphism.
- Show that this homomorphism transposes to a Lie algebra and hence Lie group homomorphism.

The effective coupling $g_{\text{eff}}(\epsilon)$ now allows for a Birkhoff decomposition in the space of formal diffeomorphisms.

Theorem 4 *Let the unrenormalized effective coupling constant $g_{\text{eff}}(\epsilon)$ viewed as a formal power series in g be considered as a loop of formal diffeomorphisms and let $g_{\text{eff}}(\epsilon) = (g_{\text{eff}_-})^{-1}(\epsilon) g_{\text{eff}_+}(\epsilon)$ be its Birkhoff decomposition in the group of formal diffeomorphisms. Then the loop $g_{\text{eff}_-}(\epsilon)$ is the bare coupling constant and $g_{\text{eff}_+}(0)$ is the renormalized effective coupling.*

The above results hold as they stand for any massless theory which provides a single coupling constant. If there are multiple interaction terms in the Lagrangian, one finds similar results relating the group of characters of the corresponding Hopf algebra to the group of formal diffeomorphisms in the multidimensional space of coupling constants.

The Role of Hochschild Cohomology

The Hochschild cohomology of the combinatorial Hopf algebras which we discuss here plays three major roles in quantum field theory:

1. it allows one to prove locality from the accompanying filtration by the augmentation degree coming from the kernels $\ker \text{Aug}^{(k)}$;

2. it allows one to write the quantum equations of motion in terms of the Hopf algebra primitives, elements in $\mathcal{H}_{\text{lin}} \cap \{\ker \text{Aug}^{(2)}/\ker \text{Aug}^{(1)}\}$; and
3. it identifies the relevant sub-Hopf algebras formed by time-ordered products.

Before we discuss these properties, let us first introduce the relevant Hochschild cohomology.

Hochschild Cohomology of Bialgebras

Let $(A, m, \mathbb{I}, \Delta, \epsilon)$ be a bialgebra, as before. We regard linear maps $L: A \rightarrow A^{\otimes n}$ as n -cochains and define a coboundary map $b, b^2 = 0$ by

$$bL := (\text{id} \otimes L) \circ \Delta + \sum_{i=1}^n (-1)^i \Delta_i \circ L + (-1)^{n+1} L \otimes \mathbb{I} \quad [55]$$

where Δ_i denotes the coproduct applied to the i th factor in $A^{\otimes n}$, which defines the Hochschild cohomology of A .

For the case $n=1$, for $L: A \rightarrow A$, [55] reduces to

$$bL = (\text{id} \otimes L) \circ \Delta - \Delta \circ L + L \otimes \mathbb{I} \quad [56]$$

The category of objects (A, C) , which consists of a commutative bialgebra A and a Hochschild 1-cocycle C on A , has an initial object $(\mathcal{H}_{\text{rt}}, B_+)$, where \mathcal{H}_{rt} is the Hopf algebra of (nonplanar) rooted trees, and the closed but nonexact 1-cocycle B_+ grafts a product of rooted trees together at a new root as described below.

The higher ($n > 1$) Hochschild cohomology of \mathcal{H}_{rt} vanishes, but in what follows, the closedness of B_+ will turn out to be crucial.

The Hopf Algebra of Rooted Trees

A rooted tree is a simply connected contractible compact graph with a distinguished vertex, the root. A forest is a disjoint union of rooted trees. Isomorphisms of rooted trees or forests are isomorphisms of graphs preserving the distinguished vertex/vertices. Let t be a rooted tree with root o . The choice of o determines an orientation of the edges of t , away from the root, say. Forests are graded by the number of vertices they contain.

Let \mathcal{H}_{rt} be the free commutative algebra generated by rooted trees. The commutative product in \mathcal{H}_{rt} corresponds to the disjoint union of trees, such that monomials in \mathcal{H}_{rt} are scalar multiples of forests. We demand that the linear operator B_+ on \mathcal{H}_{rt} , defined by

$$B_+(\mathbb{I}) = \bullet \quad [57]$$

$$B_+(t_1 \dots t_n) = \begin{array}{c} \bullet \\ \diagup \quad \diagdown \\ t_1 \quad \dots \quad t_n \end{array} \quad [58]$$

is a Hochschild 1-cocycle, which makes \mathcal{H}_{rt} a Hopf algebra. The resulting coproduct can be described as follows:

$$\Delta(t) = \mathbb{I} \otimes t + t \otimes \mathbb{I} + \sum_{\text{adm } c} P_c(t) \otimes R_c(t) \quad [59]$$

where the sum goes over all admissible cuts of the tree t . Such a cut of t is a nonempty set of edges of t that are to be removed. The forest which is disconnected from the root upon removal of those edges is denoted by $P_c(t)$ and the part which remains connected to the root is denoted by $R_c(t)$. A cut $c(t)$ is admissible if, for each vertex l of t , it contains at most one edge on the path from l to the root.

This Hopf algebra of nonplanar rooted trees is the universal object after which all such commutative Hopf algebras \mathcal{H} providing pairs (\mathcal{H}, B) , for B a Hochschild 1-cocycle, are formed.

Theorem 5 *The pair $(\mathcal{H}_{\text{rt}}, B_+)$, unique up to isomorphism, is universal among all such pairs. In other words, for any pair (\mathcal{H}, B) where \mathcal{H} is a commutative Hopf algebra and B a closed nonexact 1-cocycle, there exists a unique Hopf algebra morphism $\mathcal{H}_{\text{rt}} \xrightarrow{\rho} \mathcal{H}$ such that $B \circ \rho = \rho \circ B_+$.*

This theorem suggests that we investigate the Hochschild cohomology of the Hopf algebras of 1PI Feynman graphs. It clarifies the structure of 1PI Green functions.

The Roles of Hochschild Cohomology

The Hochschild cohomology of the Hopf algebras of 1PI graphs sheds light on the structure of 1PI Green function in at least four different ways:

- it gives a coherent proof of locality of counterterms – the very fact that

$$[Z^I, D_I] = 0 \quad [60]$$

means that the coefficients in the Lagrangian remain independent of momenta, and hence the Lagrangian remains a polynomial expression in fields and their derivatives;

- the quantum equation of motions takes a very succinct form, identifying the Dyson kernels with the primitives of the Hopf algebra;
- sub-Hopf algebras emerge from the study of the Hochschild cohomology, which connects the representation theory of these Hopf algebras to the structure of theories with internal symmetries; and
- these Hopf algebras are intimately connected to the structure of transcendental functions, such as

the generalized polylogarithms, which play a prominent role these days ranging from applied particle physics to recent developments in mathematics.

To determine the Hochschild 1-cocycles of some Feynman graph Hopf algebra \mathcal{H} , one determines first the primitives graphs γ of the Hopf algebra, which, by definition, fulfill the condition

$$\Delta(\gamma) = \gamma \otimes \mathbb{I} + \mathbb{I} \otimes \gamma \quad [61]$$

Using the pre-Lie product above, one then determines the maps

$$B_+^\gamma : \mathcal{H} \rightarrow \mathcal{H}_{\text{lin}} \quad [62]$$

such that

$$B_+^\gamma(h) = B_+^\gamma(h) \otimes \mathbb{I} + (\text{id} \otimes B_+^\gamma)\Delta(h) \quad [63]$$

where $B_+^\gamma(h) = \sum_{\Gamma} n(\gamma, h, \Gamma) \Gamma$. The coefficients $n(\gamma, h, \Gamma)$ are closely related to the section coefficients noted earlier.

Using the definition of the Bogoliubov map $\bar{\phi}$, this immediately shows that

$$S_R^\phi(B_+^\gamma(h)) = \int D_\gamma \leftarrow_{G_i} \phi_R(h) \quad [64]$$

which proves locality of counter-terms upon recognizing that B_+^γ increases the augmentation degree. Here, the insertion of the functions for the subgraph is achieved using the relevant gluing data of [36].

To recover the quantum equation of motions from the Hochschild cohomology, one proves that

$$\Gamma^\varepsilon = 1 + \sum_{\gamma} \frac{g^\gamma}{\text{Sym}(\gamma)} B_+^\gamma(X_\gamma) \quad [65]$$

where

$$X_\gamma = \prod_{e \in \gamma^{[1]_{\text{int}}}} \prod_{v \in \gamma^{[0]}} \frac{\Gamma_v^\varepsilon}{\Gamma_e^\varepsilon} \quad [66]$$

has the required solution. Upon application of the Feynman rules, the maps B_+^γ turn into the integral kernels of the usual Dyson–Schwinger equations. This allows for new nonperturbative approaches which are a current theme of investigation.

Finally, we note that the 1-cocycles introduced above allow one to determine sub-Hopf algebras of the form

$$\Delta(c_n^\varepsilon) = \sum P(\{c_j^\varepsilon\}) \otimes c_j^\varepsilon \quad [67]$$

where the c_j^ε are defined in eqn [3]. These algebras do not necessitate the considerations of single

Feynman graphs any longer, but allow one to establish renormalization directly for the sum of all graphs at a given loop order. Hence, they establish a Hopf algebra structure on time-ordered products in momentum space. For theories with internal symmetries, one expects and indeed finds that the existence of these subalgebras establishes relations between graphs that are same as the Slavnov–Taylor identities between the couplings in the Lagrangian.

Outlook

Thanks to the Hopf and Lie algebra structures described above, quantum field theory has started to reveal its internal mathematical structure in recent years, which connects it to a motivic theory and arithmetic geometry. Conceptually, quantum field theory has been the most sophisticated means by which a physicist can describe the character of the physical law. We have slowly begun to understand that, in its short-distance singularities, it encapsulates concepts of matching beauty. We can indeed expect local point-particle quantum field theory to remain a major topic of mathematical physics investigations in the foreseeable future.

See also: Bicrossproduct Hopf Algebras and Noncommutative Spacetime; Exact Renormalization Group; Hopf Algebras and q-Deformation Quantum Groups; Number Theory in Physics; Operads; Perturbation Theory and Its Techniques; Renormalization: General Theory; von Neumann Algebras: Introduction, Modular Theory, and Classification Theory.

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Hopf Algebras and q -Deformation Quantum Groups

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Introduction

Quantum groups are a remarkable generalization of conventional groups using an algebraic language by now quite well known to mathematical physicists. This language is first and foremost the concept of a “Hopf algebra.” In fact, the axioms of a Hopf algebra are so attractive from a mathematical point of view that they were proposed in the 1940s long before the advent of truly representative examples, which did not come until the 1980s (from mathematical physics). Until then, they were used mainly by mathematicians as a way for redoing group theory and Lie algebra theory in a more uniform way.

It is remarkable that at least three points of view lead to the same axioms of a Hopf algebra:

1. *Generalized symmetry* A generalization of a usual group algebra or enveloping algebra of a Lie algebra that can nevertheless act on other algebraic objects. The structure that controls this is the “coproduct” $\Delta: H \rightarrow H \otimes H$, while the group or Lie structure is encoded in the algebra H which is typically not changed up to isomorphism. Δ allows H to act on tensor products and this is needed to define what it means, for example, for a product $A \otimes A \rightarrow A$ of an algebra to be an intertwiner. The usual flip map between two representations $V \otimes W \rightarrow W \otimes V$ is not typically an intertwiner any more, instead that is provided by an R -matrix solving the Yang–Baxter equations (YBE).
2. *Noncommutative geometry* A generalization of the coordinate algebra of functions on a conventional group to allow noncommutative or “quantum” coordinate algebras. Here the group structure is encoded in a coproduct $\Delta: H \rightarrow H \otimes H$ in a way which would, in the case of functions on a group, be defined by the group product. It is typically not changed, the change being in the algebra.
3. *Duality* An object that admits observer–observed duality or Fourier transform. Such a duality is known for abelian groups, lost for nonabelian groups but re-emerges for Hopf algebras. If there is to be an algebra with product $H \otimes H \rightarrow H$, then there should also be a

“coproduct” $\Delta: H \rightarrow H \otimes H$ to maintain the duality symmetry. Then a suitable dual space H^* is also a Hopf algebra, with the roles of product and coproduct interchanged.

In line with these main ideas are three known classes of true quantum groups, and these remain the main types of example at the time of writing: the q -deformed enveloping algebras $U_q(g)$ of Drinfeld and Jimbo, their duals as quantizations of the Drinfeld–Sklyanin Poisson bracket on a simple Lie group (both of these arising from quantum inverse scattering but also in the case of $C_q[SU_2]$ from C^* -algebras) and the bicrossproduct quantum groups based on Lie group factorizations (arising from ideas for Planck-scale physics and quantum gravity). The latter are self-dual and hence are both generalized symmetries and noncommutative or quantum geometries at the same time. The impact of such quantum groups has been very far reaching from a mathematician’s point of view, spanning revolutions in the theory of knot and 3-manifold invariants, Poisson geometry, new directions in noncommutative geometry, to name some. In physics they are, at the time of writing, beginning seriously to be applied in a variety of contexts beyond the original ones, such as in book-keeping overlapping divergences in general quantum field theories, quantum computing, and construction of anyons. This article will mention some of these, but just as groups have many different roles in physics, one can expect that quantum groups and variants of them can and will have diverse roles as well. What follows is a short overview.

Hopf Algebras and First Examples

The general theory works over any field k but (to be concrete) we write our examples over \mathbb{C} ; one can also have examples over, say, the field \mathbb{Z}_2 of two elements. A Hopf algebra then is:

1. An algebra H with unit which is also a “coalgebra” with counit, that is, there are maps $\Delta: H \rightarrow H \otimes H$, $\epsilon: H \rightarrow k$ obeying:

$$(\Delta \otimes \text{id})\Delta = (\text{id} \otimes \Delta)\Delta$$

$$(\epsilon \otimes \text{id})\Delta = (\text{id} \otimes \epsilon)\Delta = \text{id}$$

2. Δ, ϵ should be algebra homomorphisms.
3. There should be a map $S: H \rightarrow H$ called the antipode or “linearized inverse” obeying

$$(\text{id} \otimes S)\Delta = (S \otimes \text{id})\Delta = 1\epsilon$$

If the third axiom is not obeyed one has a “quantum semigroup” or “bialgebra.” Note also that S looks nothing like a usual inverse and it is not, yet it plays the same role. For example, we can define conjugation or the “adjoint action” of any Hopf algebra on itself by

$$\text{Ad}_a(b) = \sum a_{(1)} b S a_{(2)}, \quad \Delta a = \sum a_{(1)} \otimes a_{(2)}$$

where we use here the “Sweedler notation” for Δa a sum of unspecified pieces in $H \otimes H$. Moreover, if it exists, then S is unique and (it can be shown) $S(ab) = (Sb)S(a)$ for all $a, b \in H$, just like an inverse.

The self-duality of these axioms is evident from the first one: a coalgebra is just an algebra with its product map $H \otimes H \rightarrow H$, unit element (viewed as a map $k \rightarrow H$ sending 1 to 1) and the associativity and unity axioms all written backwards. Meanwhile, the middle axiom means in explicit terms $\Delta(ab) = (\Delta a)(\Delta b)$, $\epsilon(ab) = \epsilon(a)\epsilon(b)$ for all $a, b \in H$ and $\Delta(1) = 1 \otimes 1$, $\epsilon(1) = 1$. This may not look self-dual but it is equivalent to saying that the product and unit are coalgebra homomorphisms. Indeed, if one takes the trouble to write out all the axioms as commutative diagrams, the set of axioms is invariant under arrow reversal. Such arrow reversal can also be concretely implemented, for example, by taking adjoints. Thus, the coproduct dualizes to a map $(H \otimes H)^* \rightarrow H^*$ and since $H^* \otimes H^* \subseteq (H \otimes H)^*$ we have a product on the dual H^* . If the dual space is defined correctly, one also has a coproduct by dualizing the product, etc. One says that two Hopf algebras H, H' are “in duality” if their maps are adjoint to each other in such a way.

The role of quantum groups as generalized symmetries is typified by the following examples. Thus, let G be a group; then its group algebra $\mathbb{C}G$ defined as a vector space (written here over \mathbb{C}) with basis identified with G and product given by the group product extended linearly, is a Hopf algebra with

$$\Delta g = g \otimes g, \quad \epsilon g = 1, \quad Sg = g^{-1}, \quad \forall g \in G$$

Likewise, if \mathfrak{g} is a Lie algebra, then its universal enveloping algebra $U(\mathfrak{g})$ generated by \mathfrak{g} is a Hopf algebra with

$$\Delta \xi = \xi \otimes 1 + 1 \otimes \xi, \quad \epsilon \xi = 0, \quad S\xi = -\xi, \quad \forall \xi \in \mathfrak{g}$$

The two examples are related if one informally allows exponentials, then $g = e^\xi$ has coproduct

$$\Delta e^\xi = e^{\Delta \xi} = e^{\xi \otimes 1 + 1 \otimes \xi} = e^\xi \otimes e^\xi$$

using axiom 2 and that $\xi \otimes 1, 1 \otimes \xi$ commute in the tensor product algebra.

The coproduct structures are therefore implicit already in Lie theory and group theory. As for any

Hopf algebra Δ , specifies how the algebra H acts in a tensor product of two representations. For groups the tensor product is diagonal (g acts on each copy), for Lie algebras it is additive (e.g., the addition of angular momenta). In general, the action of $a \in H$ is defined as the action of Δa on the tensor product. This has far-reaching consequences. For example, for the product $A \otimes A \rightarrow A$ of an algebra to be covariant means that H acting before and after the product map gives the same answer, similarly for the unit map where k has the trivial representation afforded by ϵ , that is,

$$h \triangleright (ab) = \sum (h_{(1)} \triangleright a)(h_{(2)} \triangleright b), \quad h \triangleright 1 = \epsilon(h)1$$

for all $a, b \in A$ and $h \in H$. What that means in the case of a group is therefore $g \triangleright (ab) = (g \triangleright a)(g \triangleright b)$ or G acts by automorphisms. What it means for a Lie algebra is $\xi \triangleright (ab) = (\xi \triangleright a)b + a(\xi \triangleright b)$, that is, \mathfrak{g} acts by derivations. This is how Hopf algebra theory unifies group theory and Lie algebra theory and potentially takes us beyond.

In another, dual, point of view, if G is a group defined by polynomial equations in \mathbb{C}^n , then the Hilbert’s “nullstellensatz” in algebraic geometry says that it corresponds algebraically to a commutative nilpotent-free algebra with n generators, called its “coordinate algebra” $H = \mathbb{C}[G]$. The group product then corresponds to Δ making $\mathbb{C}[G]$ into a Hopf algebra. If one replaces \mathbb{C} by any field, one has an algebraic group over the field. For example, the group $\text{SL}_2(\mathbb{C}) \subset \mathbb{C}^4$ has coordinate algebra generated by four functions a, b, c, d where a at matrix $g \in \text{SL}_2(\mathbb{C})$ has value g_{11} the 1,1 entry of the matrix, similarly $b(g) = g_{12}$ etc. Then $\mathbb{C}[\text{SL}_2]$ is the commutative algebra generated by a, b, c, d with the relation $ad - bc = 1$. A little thought about matrix multiplication should convince the reader that

$$\Delta \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \otimes \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

where we have written the operation on each generator as an array and where matrix multiplication is understood (so $\Delta a = a \otimes a + b \otimes c$, etc.). The counit and antipode are

$$\epsilon \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ S \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

One could also let G be a finite group, in which case the algebra $\mathbb{C}(G)$ of (say complex-valued) functions on it is more obviously a Hopf algebra with

$$(\Delta a)(g, h) = a(gh), \quad \epsilon(a) = a(1), \quad (Sa)(g) = a(g^{-1})$$

for any function $a \in \mathbb{C}(G)$. Here we identify $\mathbb{C}(G) \otimes \mathbb{C}(G) = \mathbb{C}(G \times G)$ or functions in two variables on the group. These examples are dually paired with $U(\mathfrak{g})$ in the Lie case and $\mathbb{C}G$ in the finite case, respectively.

In such a coordinate algebra point of view, usual constructions in group theory appear expressed backwards with arrows reversed. So an action of the group appears for such a Hopf algebra H as a “coaction” $\Delta_R: V \rightarrow V \otimes H$ (here a right coaction, one can similarly have Δ_L a left coaction). It obeys

$$(\Delta_R \otimes \text{id})\Delta_R = (\text{id} \otimes \Delta)\Delta_R, \quad (\text{id} \otimes \epsilon)\Delta_R = \text{id}$$

which are the axioms of an algebra acting written backwards for the coalgebra of H “coacting.” An example is the right action of a group on itself which in the coordinate ring point of view is $\Delta_R = \Delta$, that is, the coproduct viewed as a right coaction. It is the algebra of H that determines the tensor product of two coactions, so, for example, A is a coaction algebra in this sense if $\Delta_R: A \rightarrow A \otimes H$ is a coalgebra and an algebra homomorphism. Similarly, in this coordinate point of view, an integral on the group means a map $\int: H \rightarrow k$ and right invariance translates into invariance under the right coaction, or

$$\left(\int \otimes \text{id}\right)\Delta = 1 \int$$

There is a theorem that such an integration, if it exists, is unique up to scale. In the finite-dimensional case it always exists, for any field k . At least in this case, let $\exp = \sum_i e_i \otimes f^i$ for a basis $\{e_i\}$ of H and $\{f^i\}$ a dual basis. Then an application of the integral is Fourier transform $H \rightarrow H^*$ defined by

$$\mathcal{F}(a) = \int \sum_i e_i a \otimes f^i$$

with properties that one would expect of Fourier transform. The inverse is given similarly the other way up to a normalization factor and using the antipode of H . This is one among the many results from the abstract theory of Hopf algebras, see Sweedler (1969) and Larson and Radford (1988) among others.

A given Hopf algebra H does not know which point of view one is taking on it; the axioms of a Hopf algebra include and unify both enveloping and coordinate algebras. So an immediate consequence is that constructions which are usual in one point of view give new constructions when the wrong point of view is taken (put another way, the self-duality of the axioms means that any general theorem has a second theorem for free, given, if we keep the interpretation of H fixed, by reversing all arrows in

the original theorem and its proof). Even the elementary examples above are quite interesting for physics if taken “upside down” in this way. For example, if G is nonabelian, then $\mathbb{C}G$ is noncommutative, so it cannot be functions on any actual group. But it is a Hopf algebra, so one could think of it as being like $\mathbb{C}(\hat{G})$, where \hat{G} is not a group but a quantum group defined as $\mathbb{C}(\hat{G}) = \mathbb{C}G$. The latter is a well-defined Hopf algebra viewed the wrong way. So this is an application of noncommutative geometry to allow nonabelian Fourier transform $\mathcal{F}: \mathbb{C}(G) \rightarrow \mathbb{C}G$. Similarly, $U(\mathfrak{g})$ is noncommutative but one could view it upside down as a quantization of $\mathbb{C}[\mathfrak{g}^*] = S(\mathfrak{g})$ (the symmetric algebra on \mathfrak{g}). To do this let us scale the generators of \mathfrak{g} so that the relations on $U(\mathfrak{g})$ have the form $\xi\eta - \eta\xi = \lambda[\xi, \eta]$ where λ is a deformation parameter. Then the Poisson bracket that this algebra quantizes (deforms) is the Kirillov–Kostant one on \mathfrak{g}^* where $\{\xi, \eta\} = [\xi, \eta]$. Here ξ, η on the left-hand side are regarded as functions on \mathfrak{g}^* , while on the right-hand side we take their Lie bracket and then regard the result as a function on \mathfrak{g}^* . Examples which have been used successfully in physics include:

$$\begin{aligned} [t, x_i] &= i\lambda x_i && \text{(bicrossproduct model } \mathbb{R}_\lambda^{1,3}) \\ [x_i, x_j] &= i2\lambda \epsilon_{ijk} x_k && \text{(spin space model } \mathbb{R}_\lambda^3) \end{aligned}$$

(summation understood over k). In both cases, we may develop geometry on these algebras using quantum group methods as if they were coordinates on a usual space (see Bicrossproduct Hopf Algebras and Noncommutative Spacetime). They are versions of \mathbb{R}^n because the coproduct which expresses the addition law on the noncommutative space is the additive one according to the above. In the second case, setting the Casimir to the value for a spin j is the quadratic relation of a “fuzzy sphere.” As algebras, the latter are just the algebras of $(2j+1) \times (2j+1)$ matrices.

Going the other way, we can take a classical coordinate ring $\mathbb{C}[G]$ and regard it upside down as some kind of group or enveloping algebra but with a nonsymmetric Δ . In the finite group case, an action of $\mathbb{C}(G)$ just means a G -grading. Here if an element v of a vector space has G -valued degree $|v|$ then $a \triangleright v = a(|v|)v$ is the action of $a \in \mathbb{C}(G)$. Alternatively, this is the same thing as a right coaction of $\mathbb{C}G$, $\Delta_R v = v \otimes |v|$. Thus, the notion of group representation and group grading are also unified. This is familiar in physics for abelian groups (a $U(1)$ action is the same thing as a \mathbb{Z} -grading) but works fine using Hopf algebra methods for nonabelian groups and beyond.

Returning to axioms, if one wants to speak of real forms and unitary representations, this corresponds, for Hopf algebras, to H a $*$ -algebra over \mathbb{C} with

$$\Delta^*(\) = \tau(* \otimes *)\Delta, \qquad * \circ S = S^{-1} \circ *$$

where τ (throughout this article) denotes transposition of tensor factors. This requires in particular that S is invertible (which is not assumed for a general Hopf algebra though it does hold in the finite-dimensional case and in all examples of interest). Thus, $\mathbb{C}[SU_2]$ denotes the above with a certain $*$ structure whereby the matrix of generators is unitary.

q-Deformation Enveloping Algebras

For a genuinely representative example of a Hopf algebra, consider, $U_q(sl_2)$ defined with noncommutative generators and relations, coproduct etc.,

$$\begin{aligned} q^{h/2}x_{\pm}q^{-h/2} &= q^{\pm 1}x_{\pm} \\ [x_+, x_-] &= \frac{q^h - q^{-h}}{q - q^{-1}} \\ \Delta x_{\pm} &= x_{\pm} \otimes q^{h/2} + q^{-h/2} \otimes x_{\pm} \\ \Delta q^{h/2} &= q^{h/2} \otimes q^{h/2} \\ \epsilon x_{\pm} &= 0, \quad \epsilon q^{h/2} = 1 \\ Sx_{\pm} &= -q^{\pm 1}x_{\pm}, \quad Sq^{h/2} = q^{-h/2} \end{aligned}$$

The actual generators here are $x_{\pm}, q^{\pm h/2}$ but the notation is intended to be suggestive: if \hbar existed and we took the limit $q \rightarrow 1$, we would have the usual enveloping algebra of the Lie algebra sl_2 . The quantum group $U_q(su_2)$ is the same with the $*$ -structure $h^* = \hbar, x_{\pm}^* = x_{\mp}$ when q is real (there are other possibilities).

Two words of warning here. Although some authors write $q = e^{\hbar/2}$, the parameter q here has little to do with quantization. In fact, the cases of direct relevance to physics are $q^{2\pi i/(2+k)}$, where k is the level of the Wess–Zumino–Witten (WZW) model in which this quantum group appears as a generalized symmetry. This quantum group also (first) appeared in the theory of exactly solvable lattice models, namely the Ising model with an applied external magnetic field: $q \neq 1$ is a measure of the resulting nonhomogeneity of the model. Its origins go further back to the algebraic Bethe ansatz and the emergence of the YBE in such models (Baxter 1982). The general $U_q(\mathfrak{g})$ emerged from this context in Drinfeld (1987) and Jimbo (1985) and the same remark applies (see Affine Quantum Groups; Yang–Baxter Equations).

The second warning is that at least informally (if one works with H and allows formal power series

etc.), the algebra here is isomorphic to usual $U(sl_2)$, that is, it looks deformed but the true deformation is not here but in the coproduct, which enters into the tensor product of representations. The latter are labeled as usual because the algebra is not really changed, for example, the unitary ones of $U_q(su_2)$ are labeled by spin. The spin- $\frac{1}{2}$ one even looks the same with x_{\pm}, \hbar represented by the standard Pauli matrices. Tensor products of representations start to look different but their multiplicities are the same as classically and if V, W are representations then $V \otimes W \cong W \otimes V$. Because the coproduct above is not symmetric in its two factors, this isomorphism $\Psi_{V,W} = \tau \circ R_{V,W}$ has $R_{V,W}$ nontrivial. From the formulas given, the reader can compute that

$$R_{1/2,1/2} = q^{-1/2} \begin{pmatrix} q & 0 & 0 & 0 \\ 0 & 1 & q - q^{-1} & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & q \end{pmatrix}$$

in a tensor product basis. For this particular quantum group, and others like it, one finds that these “ R -matrices” obey the braid relations as a version of the YBE. As a result, they can and do lead to knot invariants; the one above leads to the Jones knot invariant as a polynomial in q . Briefly, one represents the knot on a plane, assigns R or R^{-1} to each braid crossing and takes a suitable trace (see The Jones Polynomial).

Since such features hold in any representation, these matrices are in fact representations of an invertible element $\mathcal{R} \in H \otimes H$ provided one allows \hbar as a generator and formal power series:

$$\mathcal{R} = q^{(h \otimes h)/2} e_{q^{-2}}^{(q - q^{-1})e \otimes f}; \quad e = x_+ q^{h/2}, \quad f = q^{-h/2} x_-$$

where

$$e_q(x) = \sum_{m=0}^{\infty} \frac{x^m}{[m]_q!}, \qquad [m]_q = \frac{1 - q^m}{1 - q}$$

are the q -exponential and q -integer, respectively. Their proper explanation is in the section “Braided groups and quantum planes.” This \mathcal{R} is called the “universal R -matrix” or quasitriangular structure and obeys

$$\begin{aligned} \tau \Delta &= \mathcal{R}(\Delta) \mathcal{R}^{-1} \\ (\Delta \otimes \text{id})\mathcal{R} &= \mathcal{R}_{13} \mathcal{R}_{23}, \qquad (\text{id} \otimes \Delta)\mathcal{R} = \mathcal{R}_{13} \mathcal{R}_{12} \end{aligned}$$

and from the axioms of a Hopf algebra, one may deduce that the YBE

$$\mathcal{R}_{12} \mathcal{R}_{13} \mathcal{R}_{23} = \mathcal{R}_{23} \mathcal{R}_{13} \mathcal{R}_{12}$$

hold in the algebra. This induces the YBE for matrices $R_{V,W}$ in the representation $V \otimes W$. Such a

Hopf algebra is called “quasitriangular” and its representations form a braided category (see Braided and Modular Tensor Categories). Even if \mathcal{R} for a quasitriangular Hopf algebra is defined by a power series, the $R_{V,W}$ in finite-dimensional representations are typically actual matrices.

Of considerable interest is the special case when q is a primitive n th root of unity. In this case the quasitriangular Hopf algebra $u_q(sl_2)$ has the above generators but the additional relations

$$e^n = f^n = 0, \quad g^n = 1; \quad g = q^b$$

which render the algebra generated by e, f, g as n^3 -dimensional. The algebra no longer has a matrix block decomposition (is not semisimple) and not all representations descend to it. For example, if n is odd, then only representations of dimension $\leq n$ descend. Other than this, one has many of the features of a classical enveloping algebra now for this finite-dimensional object. There is evidence that such objects over \mathbb{C} are intimately related to classical Lie algebras but over a finite field.

Finally, there is a similar theory of $U_q(\mathfrak{g})$ for all Lie algebras determined by symmetrizable Cartan matrices $\{a_{ij}\}$, including affine ones. Here $i, j \in I$ an indexing set and $a_{ij} = 2i \cdot j / i \cdot i \in \{0, -1, -2, \dots\}$ for $i \neq j$, where \cdot is a symmetric bilinear form on the root lattice $\mathbb{Z}[I]$ generated by I with $i \cdot i$ a positive even integer. To be precise, one should also fix a “root datum” in the form of an inclusion $\mathbb{Z}[I] \subseteq X$ of the root lattice into a choice of character lattice X and an inclusion $\mathbb{Z}[I] \subseteq Y$ of the coroot lattice (also labeled by I) into the cocharacter lattice Y (the dual of X). Here the evaluation pairing is required to restrict to $\langle i^\sim, j \rangle = a_{ij}$ if $i, j \in I$ and i^\sim is i viewed in the cocharacter lattice Y . We let $q_i = q^{i \cdot i/2}$ and require $q_i^2 \neq 1$ for all i (or one may consider q as an indeterminate). We have generators e_i, f^i for $i \in I$ and invertible g_a for a each generator of Y , and the relations

$$\begin{aligned} g_a e_i &= q^{(a,i)} e_i g_a, & f^i g_a &= q^{(a,i)} g_a f^i \\ [e_i, f^j] &= \frac{g_i^{i \cdot i/2} - g_i^{-i \cdot i/2}}{q_i - q_i^{-1}} \delta_i^j \\ \sum_{r=0}^{1-a_{ij}} (-1)^r \binom{1-a_{ij}}{r}_{q_i} (e_i)^r e_j (e_i)^{1-a_{ij}-r} &= 0 \end{aligned}$$

for all $i \neq j$ and an identical set for the $\{f^i\}$. The coalgebra and antipode are

$$\begin{aligned} \Delta e_i &= e_i \otimes g_i^{i \cdot i/2} + 1 \otimes e_i \\ \Delta f^i &= f^i \otimes 1 + g_i^{-i \cdot i/2} \otimes f^i \\ \Delta g_a &= g_a \otimes g_a, \quad \epsilon(g_a) = 1, \quad \epsilon(e_i) = \epsilon(f^i) = 0 \\ S g_a &= g_a^{-1}, \quad S e_i = -e_i g_i^{-i \cdot i/2}, \quad S f^i = -g_i^{i \cdot i/2} f^i \end{aligned}$$

The q -Serre relations are those above involving the q -binomial coefficients, defined now using the symmetric q -integers $(m)_q = (q^m - q^{-m})/(q - q^{-1})$. They have their true explanation as

$$\text{Ad}_{(e_i)^{1-a_{ij}}}(e_j) = 0$$

where Ad is a braided group adjoint action in the sense of the section “Braided groups and quantum planes.” Notice that while the root generators are modeled on the Lie algebra, the Cartan generators are modeled on the torus of an algebraic group, which contains global information. Thus, the more precise form of $U_q(sl_2)$ is the e, f, g form with the generator $g = q^b$ as above, with $\mathbb{Z}[I] \subsetneq X$ and $\mathbb{Z}[I] = Y$. Meanwhile $U_q(psl_2)$ has the square root of this as generator (what we called $q^{b/2}$ before) with $\mathbb{Z}[I] = X$ and $\mathbb{Z}[I] \subsetneq Y$ where the strict inclusion has $1=2$ in the lattice \mathbb{Z} . Note that, in the complex case, SL_2 has compact real form SU_2 while its quotient, PSL_2 , has compact real form SO_3 , so these are distinguished at the Hopf algebra level. In general, the root datum has an associated reductive algebraic group which is simply connected when $Y = \mathbb{Z}[I]$ and generated by its adjoint representation when $X = \mathbb{Z}[I]$. The complexified character lattice is a sublattice of the more familiar Lie algebra weight lattice and labels representations that extend to the (algebraic) group. Langlands duality interchanges the roles of X, Y . These subtleties are lost when we work over formal power series with $q = e^{\lambda/2}$ and Lie-algebra-like Cartan generators.

These objects are mathematically so interesting that some authors define “quantum groups” as nothing more than this particular extension of the theory of Lie algebras, Cartan matrices and root systems. Among the deepest theorems is the existence of the Lusztig–Kashiwara canonical basis which is obtained from $q=0$ but valid also at $q=1$ (i.e., for classical enveloping algebras) and which has the remarkable property of inducing bases coherently across highest-weight representations. From a physicist’s point of view, however, there are many other Hopf algebras rather more closely connected with actual quantization. Most often, the terms quantum group and Hopf algebra are used interchangeably.

There is similarly a reduced version $u_q(\mathfrak{g})$. The simplest of all possible cases, even simpler than $u_q(sl_2)$, is for what one could call $u_q(1)$ with a single generator g and

$$g^n = 1, \quad \Delta g = g \otimes g, \quad \epsilon g = 1, \quad S g = g^{-1}$$

$$\mathcal{R}_q = \frac{1}{n} \sum_{a,b=0}^{n-1} q^{-ab} g^a \otimes g^b$$

where q is a primitive n th root of unity. The Hopf algebra is the same as the group algebra $\mathbb{C}Z_n = \mathbb{C}(\hat{Z}_n)$ but the \mathcal{R} is nontrivial. A representation means a \hat{Z}_n -graded space, that is, graded into degrees $0, 1, \dots, n-1$. The braiding matrices have the diagonal form $R_{V_a, W_b} = q^{ab}$ on components of degree a, b , respectively. The braided category generated in this case is the one where anyons live. From this point of view, $u_q(g)$ generate the category where nonabelian anyons live. Here \mathcal{R}_{q^2} (in place of $q^{(b \otimes b)/2}$) along with an additional $e_{q^{-2}}$ factor as above gives the quasitriangular structure of $u_q(sl_2)$. The physical model here is the rational conformal field theory mentioned above with these anyons as particular bound states. There is a proposal to use them in the construction of quantum computers.

q -Deformation Coordinate Algebras

From the coordinate algebra point of view, the corresponding deformation to the one in the last section is the Hopf algebra $\mathbb{C}_q[SL_2]$ with noncommuting generators and relations

$$\begin{aligned} ca &= qac, & ba &= qab \\ db &= qbd, & dc &= qcd \\ bc &= cb, & da - ad &= (q - q^{-1})bc \\ ad - q^{-1}bc &= 1 \end{aligned}$$

The coalgebra has the same matrix form on the generators as for $\mathbb{C}[SL_2]$ and the antipode and $*$ -structure (for $\mathbb{C}_q[SU_2]$) are

$$S\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} d & -qb \\ -q^{-1}c & a \end{pmatrix} = \begin{pmatrix} a & c \\ b & d \end{pmatrix}^*$$

Its duality pairing with $U_q(sl_2)$ is afforded by the 2×2 Pauli-matrix representation of the latter. The $\mathbb{C}_q[SU_2]$ Hopf $*$ -algebra may be completed to a C^* -algebra.

One similarly has $\mathbb{C}_q[G]$ for all semisimple Lie groups G and their various real forms. From an axiomatic point of view, such quantum groups are “coquasitriangular” in the sense that there is a map $\mathcal{R}: H \otimes H \rightarrow k$ such that

$$\sum \mathcal{R}(a_{(1)} \otimes b_{(1)}) a_{(2)} b_{(2)} = \sum b_{(1)} a_{(1)} \mathcal{R}(a_{(2)} \otimes b_{(2)})$$

for all $a, b \in H$ and

$$\begin{aligned} \mathcal{R}(ab \otimes c) &= \sum \mathcal{R}(a \otimes c_{(1)}) \mathcal{R}(b \otimes c_{(2)}) \\ \mathcal{R}(a \otimes bc) &= \sum \mathcal{R}(a_{(1)} \otimes c) \mathcal{R}(a_{(2)} \otimes b) \end{aligned}$$

for all $a, b, c \in H$. We also require that \mathcal{R} is invertible in a certain sense. These are just the arrow reversal of the axioms of a quasitriangular

structure. In general, for the deformation of a linear algebraic group we will have some n^2 generators t^i_j , now taken to be noncommutative, and with a matrix form of coalgebra

$$\Delta t^i_j = t^i_k \otimes t^k_j, \quad \epsilon t^i_j = \delta^i_j$$

For the compact real form we will have $St^i_j = t^{i*}_j$. Moreover, from the first of the above axioms we will have among the relations

$$R^i_k t^a_j t^b_l = t^k_b t^i_a R^a_b l$$

where $R^i_k = \mathcal{R}(t^i_j \otimes t^k_l)$ is a matrix $R \in M_n \otimes M_n$ obeying the YBE. If we take only these quadratic relations, we have the “Faddier Reshetikhin Takhtajan (FRT) bialgebra” $A(R)$ and it can be shown (see Majid 1995) that R extends to a coquasitriangular structure \mathcal{R} on it. However, in our case we also have

$$\begin{aligned} R^{-1i}_j t^k_l &= \mathcal{R}(St^i_j \otimes t^k_l) \\ \tilde{R}^i_k t^j_l &= \mathcal{R}(t^i_j \otimes St^k_l) \end{aligned}$$

where $\tilde{R} = ((R^{t_2})^{-1})^{t_2}$ (t_2 transposition in the second factor of M_n) is called the “second inverse” of R . With these additional matrices, one may define a q -determinant and antipode relations as well (Majid 1995). One may also generate a rigid braided monoidal category and reconstruct a Hopf algebra $\tilde{A}(R)$ from it. In this way, the R -matrix plays a role similar to that of the structure constants of a Lie algebra and can in principle define the quantum group coordinate algebra. Such R -matrices have been classified in low dimension and include multiparameter and other deformations of classical group coordinate algebra as well as other nonstandard quantum groups.

In the $\mathbb{C}_q[G]$ examples it is not the coalgebra which is essentially deformed but the algebra. We already see this above on the generators but the coproduct of a product of generators may look different. Nonetheless, one can identify the vector space that the products generate with that of $\mathbb{C}[G]$ and at least informally with respect to a deformation parameter express the product as a power series in the undeformed product (a \bullet -product deformation). For generic values, one still has a Peter–Weyl decomposition $\mathbb{C}_q[G] = \oplus (V \otimes V^*)$, where the sum is over irreducibles corepresentations, which can be identified with the classical representations of the algebraic group. One can make the same decomposition for $\mathbb{C}[G]$ and identify the matrix blocks $V \otimes V^*$ in order to find this \bullet -product. Also, since this is a flat deformation, it follows that the commutator at lowest order defines a Poisson bracket on G , given by

$$\{t^i_j, t^k_l\} = t^i_a t^k_b r^a_b l - r^i_a k b t^a_j t^b_l$$

and this Poisson bracket is compatible with the group product $G \times G \rightarrow G$ as a Poisson map (because the Hopf algebra coproduct was an algebra map). Here r is the first order part in the expansion of the R -matrix. A Lie group equipped with a Poisson bracket compatible in this way is called a “Poisson Lie group.” On general functions its Poisson bivector is generated by the first order part $r \in \mathfrak{g} \otimes \mathfrak{g}$ in the expansion of \mathcal{R} in the q -deformed enveloping algebra. In place of the YBE obeyed by \mathcal{R} , we have the “classical Yang–Baxter equations (CYBE),”

$$[r_{12}, r_{23}] + [r_{12}, r_{13}] + [r_{13}, r_{23}] = 0$$

In this way, one may characterize an “infinitesimal version” of $U_q(\mathfrak{g})$ as $(\mathfrak{g}, r, \delta)$ where $\delta: \mathfrak{g} \rightarrow \mathfrak{g} \otimes \mathfrak{g}$ is the leading part of $\tau\Delta - \Delta$ and makes the triple into a quasitriangular “Lie Bialgebra” (see Classical r -Matrices, Lie Bialgebras, and Poisson Lie Groups).

Finally, returning to our example, when q is an n th root of unity, one has the q -Frobenius Hopf algebra homomorphism

$$\begin{aligned} \mathbb{C}[SL_2] &\hookrightarrow \mathbb{C}_q[SL_2] \\ \begin{pmatrix} a & b \\ c & d \end{pmatrix} &\mapsto \begin{pmatrix} a^n & b^n \\ c^n & d^n \end{pmatrix} \end{aligned}$$

that is, a classical copy sitting inside the quantum group. Quotienting by this means adding the relations

$$a^n = d^n = 1, \quad b^n = c^n = 0$$

which gives the finite-dimensional reduced quantum group $\mathbb{C}_q^{\text{red}}[SL_2]$. Similarly for other $\mathbb{C}_q^{\text{red}}[G]$. These reduced quantum groups provide finite noncommutative geometries having the geometric flavor of the classical geometry but where geometry and physics (such as electromagnetic gauge theory modes) are fully computable.

Self-Dual Quantum Groups

The arrow-reversibility of the axioms of a quantum group make it possible to search for self-dual quantum groups or for quantum groups which, if not self-dual, have a self-dual form. This leads to the bicrossproduct quantum groups coming from models of quantum gravity (Majid 1988) (see Bicrossproduct Hopf Algebras and Noncommutative Spacetime).

The context here is that of Figure 1 which shows how Hopf algebras relate to other objects and to duality in a representation-theoretic sense. Along the central axis, we have put self-dual categories or in physical terms categories admitting Fourier transform. This is clear for abelian Groups where the

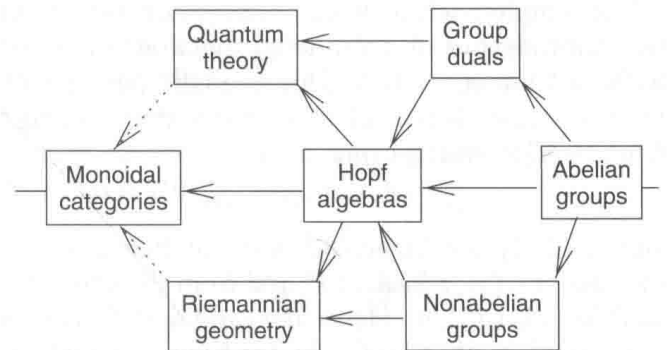


Figure 1 Role of Hopf algebras along the self-dual axis.

dual \hat{G} of an abelian group G is also an abelian group. Below the axis, we have nonabelian groups which we view as toy models of geometries with curvature. Every compact Lie group, for example, has an associated Killing metric. Above the axis, a nonabelian group dual \hat{G} means to construct unitary representations etc., which we view as toy models of quantum theory. We have seen that Hopf algebras are another self-dual category and provide a framework in which both groups and group duals can be unified (see the section “Hopf algebras and first examples”). Thus, G can be viewed as a coordinate Hopf algebra $\mathbb{C}(G)$ or $\mathbb{C}[G]$ in the finite or Lie cases, and \hat{G} as the dual Hopf algebra $\mathbb{C}G$ or $U(\mathfrak{g})$ as a definition of the coordinate algebra “ $\mathbb{C}(\hat{G})$.” Note that \hat{G} is not merely the set of representations, as these alone are not enough to reconstruct the group (e.g., both S^1 and SO_3 have the same set). We see that Hopf algebras are a microcosm for the unification of quantum theory and gravity. Hopf algebra duality interchanges the role of position and momentum on the one hand and of quantum and gravitational effects on the other. A self-dual Hopf algebra has both aspects unified and interchanged by the self-duality.

One can also ask what the next most general self-dual category of objects is in which to look for more general unifications. One answer here is the category whose objects are themselves categories \mathcal{C} equipped with a tensor product (a “monoidal category”) and a monoidal functor to a fixed monoidal category \mathcal{V} . Motivated by the above, a theorem from the 1980s is that for any such \mathcal{C} there is a dual \mathcal{C}^0 of “representations in \mathcal{V} ” (Majid 1991a). The dotted arrows in Figure 1 indicate that this may be a setting for more ambitious models than those achieved by Hopf algebras alone. In fact, the \mathcal{C}^0 construction was one of the ingredients going into the invention of 2-categories a few years later. See also several articles on TQFT (such as Topological Quantum Field Theory: Overview; Axiomatic Approach to Topological Quantum Field Theory; Duality in Topological Quantum Field Theory).

The simplest self-dual quantum group is $\mathbb{C}[x]$ as the Hopf algebra of polynomial functions on a line with additive coproduct. This is dually paired with itself in the form of the enveloping algebra $U(\mathfrak{gl}_1) = \mathbb{C}[p]$ with pairing

$$\langle p^m, x^n \rangle = (-i)^n \delta_{m,n} n!$$

and similarly for higher-dimensional flat space. In the case of $\mathbb{C}[x]$, a basis is x^n and from the above the dual basis is $(ip)^n/n!$. Hence the canonical element is $\exp = e^{ix \otimes p}$ so that Hopf algebra Fourier transform on a suitable completion of these algebras reduces to usual Fourier transform.

A more nontrivial example (Majid 1988) is given by the “Planck-scale Hopf algebra” $\mathbb{C}[x] \bowtie \mathbb{C}[p]$ which has algebra and coalgebra

$$\begin{aligned} [p, x] &= i\hbar(1 - e^{-\gamma x}), & \Delta x &= x \otimes 1 + 1 \otimes x \\ \Delta p &= p \otimes e^{-\gamma x} + 1 \otimes p, & \epsilon x &= \epsilon p = 0 \\ Sx &= -x, & Sp &= -pe^{\gamma x} \end{aligned}$$

The actual generator here should be $e^{\gamma x}$ rather than x for an algebraic treatment (otherwise one should allow power series or use C^* -algebras). The dually paired Hopf algebra has the same form $\mathbb{C}[p] \bowtie \mathbb{C}[x]$, with new parameters $\hbar' = 1/\hbar$ and $\gamma' = \hbar\gamma$ and quantum group Fourier transform connects the two. More details and the general construction of Hopf algebras $\mathbb{C}[M] \bowtie U(\mathfrak{g})$ with dual $U(\mathfrak{m}) \bowtie \mathbb{C}[G]$ are in the article on “bicrossproduct” Hopf algebras (see Bicrossproduct Hopf Algebras and Noncommutative Spacetime). These quantize particles in M moving under momentum Lie group G with Lie algebra \mathfrak{g} and vice versa. The states of one (in a C^* -algebra context) lie in the algebra of observables of the other (“observable–state duality”). The data required are a matched pair of actions of (G, M) on each other. Such equations correspond locally to a factorization of a larger group $G \bowtie M$ but typically have singularities and other features in keeping with a toy model of Einstein’s equations.

There are, by the time of writing, many applications of bicrossproducts beyond the original one, including a Poincaré quantum group for the $\mathbb{R}_\lambda^{1,3}$ mentioned in the section “Hopf algebras and first examples,” with links to Planck-scale physics. There is also a bicrossproduct quantum group $\mathbb{C}[G^*] \bowtie U(\mathfrak{g})$ canonically associated to any simple Lie algebra \mathfrak{g} and related to T -duality. The classical data here are Lie bialgebras and solutions of the CYBE as in the section “ q -Deformation coordinate algebras,” however there is no known relation with the q -deformation Hopf algebras themselves. Finite group bicrossproducts are also interesting and examples (but not with both actions nontrivial) were already in the works of GI Kac in the 1960s.

These constructions also work when the groups above are themselves Hopf algebras. For example, any finite-dimensional Hopf algebra H has a “quantum double” $D(H) = H \bowtie H^{*\text{op}}$, where the double cross product \bowtie is by mutual coadjoint actions. The cross-relations between the two sub-Hopf algebras are

$$\sum \langle h_{(1)}, a_{(1)} \rangle h_{(2)} a_{(2)} = \sum a_{(1)} h_{(1)} \langle h_{(2)}, a_{(2)} \rangle$$

for $h \in H$ and $a \in H^*$. The construction is due to Drinfeld (1987) while the \bowtie form is due to the author. Moreover, $D(H)$ is quasitriangular with $\mathcal{R} = \exp$, the canonical element used in the Fourier transform on H . Its representations consist of vector spaces where H acts and at the same time $H^{*\text{op}}$ acts or (which makes sense when H is infinite dimensional) where H coacts, in a compatible way. Such objects are called “crossed modules” because when $H = CG$, one has exactly a linearization of the crossed G -sets of JC Whitehead. They are a special case of the \mathcal{C}^0 construction mentioned above.

Finally, one can also view the q -deformed linear spaces on which quantum groups such as $U_q(\mathfrak{g})$ act as self-dual Hopf algebras under an additive coproduct. However, this needs to be as braided groups or Hopf algebras with braid statistics, see the next section. The simplest example here is the “braided line” $B = \mathbb{C}[x]$ developed not as above but as a self-dual Hopf algebra with q -statistics. Its “bosonization” gives a self-dual Hopf algebra $U_q(b_+) \subset U_q(\mathfrak{sl}_2)$, and similarly for other $U_q(b_+) \subset U_q(\mathfrak{g})$. Perhaps more surprisingly, the quantum groups $U_q(\mathfrak{g})$ and $C_q[G]$ also both have canonical braided group versions (a process called “transmutation”) and as such they too are isomorphic. This isomorphism extends the linear isomorphism $\mathfrak{g} \rightarrow \mathfrak{g}^*$ afforded by the Killing form of any semisimple Lie algebra. In physical terms, what this means is that there is in q -deformed geometry just one self-dual object $B_q(G)$ with two different scaling limits

$$U(\mathfrak{g}) \longleftarrow B_q(G) \rightarrow \mathbb{C}[G]$$

as $q \rightarrow 1$, and the structure of which underlies the deeper structure of $U_q(\mathfrak{g})$ and $C_q[G]$ as well.

Braided Groups and Quantum Planes

A super quantum group or super-Hopf algebra is not a quantum group or Hopf algebra since the key homomorphism property of $\Delta: H \rightarrow H \otimes H$ is modified: one must use in the target $H \otimes H$ the \mathbb{Z}_2 -graded or super tensor product of super algebras. Here,

$$(a \otimes b)(c \otimes d) = (-1)^{|b||c|} ac \otimes bd$$

for elements of degree $|b|, |c|$. Super quantum groups $U_q(gl_m|n)$ etc., have been constructed and have an analogous theory to the bosonic versions above. Super spaces in physics are associated to differential forms and in the same way a bicovariant exterior algebra on a quantum group H is generally a super quantum group. Here the exterior algebra is generated on by 1-forms and the coproduct on 1-forms is

$$\underline{\Delta} = \Delta_L + \Delta_R$$

Here $\Delta_{L,R}$ are the coactions of H on 1-forms induced by the left and right coaction of H on itself.

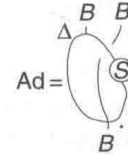
For a true understanding of quantum groups one must, however, go beyond such objects to “braided groups” or Hopf algebras with braid statistics (see Majid 1995). This theory was introduced by the author in the early 1990s as a more systematic method for q -deformation of structures in physics based on q -group covariance. We have seen that a quasitriangular quantum group, or any Hopf algebra through its double, generates a braided category with the flip map τ replaced by a braiding $\Psi_{V,W}$ between any two representations. Anything which is covariant under the quantum group means by definition that it lives in the braided category. Working with such “braided algebras” is similar to working with superalgebras except that one should use Ψ in place of the graded transposition in any algebraic construction. In particular, two braided algebras have a natural “braided tensor product” also in the category. In concrete terms,

$$(a \otimes b)(c \otimes d) = a\Psi(b \otimes c)d$$

Then a Hopf algebra in the braided category or braided group is B , an algebra in the category along with a coalgebra and antipode, where $\underline{\Delta}: B \rightarrow B \otimes B$ is an algebra homomorphism (see Braided and Modular Tensor Categories).

Next, we have mentioned in the section “ q -Deformation enveloping algebras” that q -algebras generate topological invariants, but we now turn this on its head and use braid diagrams to do q -algebra. We write all operations as flowing down the page, any transpositions in the algebraic construction are expressed as a braid crossing $\Psi = \times$ or its inverse by the reversed braid crossing, and any other operations as nodes. Thus, a product is denoted Υ and a coproduct λ . Algebraic information “flows” along these “wires” much like the way that information flows along the wiring in a computer, except that under- and over-crossings represent distinct nontrivial operators. (In fact, one may formulate topological quantum computers exactly in this way.) In this notation, tensor

products are denoted by juxtaposition and the trivial object in the category is omitted. In particular, one has the axioms and all general theorems of Hopf algebras at this diagrammatic level. For example, the adjoint action of any braided group B on itself is (see Majid 1995)



In any concrete example, such diagrams turn into R -matrix formulas where $\Psi = \tau R$ as explained in the section “ q -Deformation enveloping algebras.”

A basic example of a braided group is the braided q -plane C_q^2 with generators x, y and relations $yx = qxy$. Its coproduct is the additive one $\underline{\Delta}x = x \otimes 1 + 1 \otimes x$ (and similarly for y) reflecting addition in the plane, but this is extended to products as a braided group with braiding $q^{1/2}R_{1/2,1/2}$ in terms of the R -matrix in the section “ q -Deformation enveloping algebras.” The extra factor here means that C_q^2 lives in the braided category of representations of $U_q(gl_2) = \tilde{U}_q(sl_2)$ (i.e., with an additional central $U_q(1)$ generator to provide the $q^{1/2}$). More precisely, the category is that of corepresentations of $C_q[GL_2] = \tilde{C}_q[SL_2]$. The coaction in this case is

$$\Delta_R(x \ y) = (x \ y) \otimes \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

where the additional central generator is encoded in the q -determinant (which is no longer set equal to 1). Notice that $q^{1/2}R_{1/2,1/2}$ has eigenvalues $q, -q^{-1}$ (one says that it is q -Hecke). Another braided group, associated now to the second eigenvalue is $C_q^{0|2}$ with generators ξ, η and relations $\eta\xi = -q^{-1}\xi\eta$, $\xi^2 = \eta^2 = 0$. It is the quadratic algebra dual of C_q^2 (Manin 1988).

One has natural braided linear spaces for the whole family $C_q[G]$, on which the latter coact after central extension. The general construction is as follows. If V is an object in a braided category (e.g., the fundamental representation of a quantum group), let $T(V)$ be the tensor algebra generated by a basis $\{e_i\}$ of V with no relations and the additive braided coproduct as above. Assume that V has a dual V^* in the category, and similarly form $T(V^*)$ with dual basis generators $\{f^i\}$. These two braided groups will be dually paired by extending the evaluation map to products, which takes the form of “braided integers” (see Majid 1995)

$$\langle f^{i_m} \cdots f^{i_1}, e_{j_1} \cdots e_{j_n} \rangle = \delta_{n,m} [n, \Psi]_{j_1 \cdots j_n}^{i_1 \cdots i_n}$$

$$[n, \Psi] = \text{id} + \Psi_{12} + \Psi_{12}\Psi_{23} + \cdots + \Psi_{12} \cdots \Psi_{n-1,n}$$

We now quotient by the kernels of this pairing to obtain $B(V), B(V^*)$ as two nondegenerately paired braided groups. This quotient generates all the relations, which are very often but not necessarily quadratic (in practice, one typically imposes only the quadratic relations to have braided groups with a possibly degenerate pairing). The construction is due to the author. Moreover, we can define partial derivatives on these braided groups by $\Delta a = 1 \otimes a + e_i \otimes \partial^i a + \dots$ for any a in the algebra, that is, as an infinitesimal generator of translations under the braided group law; similarly exp, indefinite and Gaussian integration, Fourier transform, etc. The simplest example here is $B = \mathbb{C}[x]$ viewed not as a usual Hopf algebra but as a braided group in the category of \mathbb{Z} -graded spaces with $\Psi(x \otimes x) = qx \otimes x$. Also in this example the braided addition law on $\mathbb{C}[x]$ is

$$\Delta x^n = \sum_{m=0}^n \begin{bmatrix} n \\ m \end{bmatrix}_q x^m \otimes x^{n-m}$$

defined by $[m]_q$, and the partial derivative defined by it is the Jackson (1908) q -derivative

$$\partial f(x) = \frac{f(x) - f(qx)}{x(1 - q)}$$

while $\Delta e_q(x) = e_q(x) \otimes e_q(x)$ if we allow power series. Such objects occur in the theory of q -special functions (see q -Special Functions).

Among deeper theorems (see Majid 1995, 2002), there is a triangular decomposition

$$U_q(\mathfrak{g}) = U_q(\mathfrak{n}_-) \bowtie T \bowtie U_q(\mathfrak{n}_+)$$

where $U_q(\mathfrak{n}_+)$ is a braided group and $U_q(\mathfrak{n}_-)$ is dually paired to its opposite. T denotes the torus generators $\{g_a\}$ in the section “ q -Deformation enveloping algebras.” More generally, if $\mathfrak{g}_0 \subset \mathfrak{g}$ is a principal embedding of Lie algebras (given by an inclusion of Dynkin diagrams), then $U_q(\mathfrak{g}) = B^* \bowtie U_q(\mathfrak{g}_0) \bowtie B^{\text{op}}$ for some additive braided group of additional root generators and its dual. The general construction $B^* \bowtie H \bowtie B^{\text{op}}$ here is “double bosonization” which associates to dual braided groups B, B^* in the category of representations of some quasitriangular Hopf algebra H , a new quasitriangular Hopf algebra. The simplest example $B = \mathbb{C}[x]$ lives in the category of representations of $T = U_q(1)$ in an algebraic form. The dual is another braided line $\mathbb{C}[p]$ and $\mathbb{C}[p] \bowtie U_q(1) \bowtie \mathbb{C}[x]$ is a version of $U_q(\mathfrak{sl}_2)$. In this way, the braided line $\mathbb{C}[x]$ is at the root of all q -deformation quantum groups.

An earlier theorem is that for any braided group B covariant under a (co)quasitriangular H , we have its ‘bosonization’ $B \bowtie H$. There is a similar “biproduct” if B lives in the category of crossed modules for any

Hopf algebra H . These have been extensively applied in physics notably in the construction of inhomogeneous quantum groups. Similar to \mathbb{C}_q^2 (but as a $*$ -algebra), there is a natural self-dual q -Minkowski space $B = \mathbb{R}_q^{1,3}$ which is covariant under $U_q(\mathfrak{so}_{1,3})$, and its bosonization is the q -Poincaré plus dilations group $\mathbb{R}_q^{1,3} \bowtie U_q(\mathfrak{so}_{1,3})$. It is not possible to avoid the dilation here. The double-bosonization extends this to the q -conformal group $U_q(\mathfrak{so}_{2,4})$. The braided adjoint action becomes the action of conformal translations on $\mathbb{R}_q^{1,3}$. The construction of q -propagators and q -deformed physics on such q -Minkowski space was achieved in the mid 1990s as one of the main successes of the theory of braided groups.

This $\mathbb{R}_q^{1,3}$ can be given also as a matrix of generators, relations, $*$ -structure and, a second braided coproduct:

$$\begin{aligned} \beta\alpha &= q^2\alpha\beta, & \gamma\alpha &= q^{-2}\alpha\gamma, & \delta\alpha &= \alpha\delta \\ \beta\gamma &= \gamma\beta + (1 - q^{-2})\alpha(\delta - \alpha) \\ \delta\beta &= \beta\delta + (1 - q^{-2})\alpha\beta \\ \gamma\delta &= \delta\gamma + (1 - q^{-2})\gamma\alpha \\ \Delta \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} &= \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \otimes \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \\ \epsilon \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, & \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}^* &= \begin{pmatrix} \alpha & \gamma \\ \beta & \delta \end{pmatrix} \end{aligned}$$

This is in addition to the additive coproduct above. It corresponds to the point of view of Minkowski space as Hermitian 2×2 matrices. Note that Δ is not a $*$ -algebra map in the usual sense and indeed Hermitian matrices are not a group under multiplication, but this does form a natural braided $*$ -bialgebra. If we quotient by the braided determinant relation $\alpha\delta - q^2\gamma\beta = 1$, we have the unit hyperboloid in $\mathbb{R}_q^{1,3}$ which turns out to be the braided group $B_q[SU_2]$ mentioned at the end of the previous section (as obtained canonically from $\mathbb{C}_q[SU_2]$). We now have a braided antipode

$$S \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} = \begin{pmatrix} q^2\delta + (1 - q^2)\alpha & -q^2\beta \\ -q^2\gamma & \alpha \end{pmatrix}$$

This was the first nontrivial example of a braided group (Majid 1991b) and we see that it has two $q \rightarrow 1$ limits

$$U(\mathfrak{su}_2) \longleftarrow B_q[SU_2] \rightarrow \mathbb{C}[\text{Hyperboloid} \subset \mathbb{R}^{1,3}]$$

Because most constructions in physics can be uniformly deformed by such methods (including the totally q -antisymmetric tensor), one finds that q provides a new regulator in which infinities in quantum field theory can be in principle be encoded as poles at $q = 1$. That transmutation from the

quantum group to its braided version unifies unitary nonabelian symmetries with pseudo-Riemannian geometry is another deeper aspect of relevance to physics. In addition, q -constructions have their original role in quantum integrable systems, at q a root of unity and for infinite-dimensional (affine) Lie algebra deformations.

Quasi-Hopf Algebras

Although the braided category of representations of a quantum group has a trivial “associator” $\Phi_{V,W,Z}: (V \otimes W) \otimes Z \rightarrow V \otimes (W \otimes Z)$ between any three objects, a general braided category and the diagrammatic methods of “braided algebra” in the last section do not require this (one simply translates diagrams into algebra by inserting Φ as needed). A more general object that generates such categories as its representations is a “quasi-Hopf algebra.” This is a generalization of Hopf algebras in which the coproduct $\Delta: H \rightarrow H \otimes H$ is not necessarily coassociative. Instead,

$$\begin{aligned}(\text{id} \otimes \Delta)\Delta &= \phi((\Delta \otimes \text{id})\Delta)\phi^{-1} \\(\text{id} \otimes \epsilon \otimes \text{id})\phi &= 1 \\ \phi_{234}(\text{id} \otimes \Delta \otimes \text{id})(\phi)\phi_{123} \\ &= (\text{id}^2 \otimes \Delta)(\phi)(\Delta \otimes \text{id}^2)(\phi)\end{aligned}$$

for some invertible element $\phi \in H \otimes H \otimes H$. The numbers denote the position in the tensor product and one says that ϕ is a 3-cocycle. The axioms for the antipode and quasitriangular structure \mathcal{R} are also modified. The tensor product of representations is given as usual by Δ , and the braiding and associator by the actions of \mathcal{R} and ϕ .

This notion, due to Drinfeld (1990), arises when one wishes to write down the quantum groups $U_q(\mathfrak{g})$ more explicitly as built on the algebras $U(\mathfrak{g})$ (recall that they are isomorphic over formal power series). Thus, for each semisimple \mathfrak{g} there is a natural (quasitriangular) quasi-Hopf algebra $(U(\mathfrak{g}), \phi, \mathcal{R})$ where $U(\mathfrak{g})$ has the usual Hopf algebra structure, \mathcal{R} is an exponential of the split Casimir (or inverse Killing form) in $\mathfrak{g} \otimes \mathfrak{g}$ and ϕ is constructed as a solution of the Knizhnik–Zamolodchikov equations coming out of conformal field theory. This is not $U_q(\mathfrak{g})$ but it has an equivalent braided category of representations. Thus, there is an element $F \in U(\mathfrak{g})^{\otimes 2}$ (extended over formal power series) such that

$$\begin{aligned}\Delta_F &= F(\Delta)F^{-1}, \quad \mathcal{R}_F = F_{21}\mathcal{R}F^{-1} \\ \phi_F &\equiv F_{12}(\Delta \otimes \text{id})(F)\phi(\text{id} \otimes \Delta)(F^{-1})F_{23}^{-1} = 1\end{aligned}$$

recovers $U_q(\mathfrak{g})$ as a quasitriangular Hopf algebra built directly on the algebra $U(\mathfrak{g})$. The conjugation

operations here (and a similar process regarding the antipode) are a “Drinfeld twist” of a quasi-Hopf algebra, and such twisting by any invertible F such that

$$(\epsilon \otimes \text{id})F = (\text{id} \otimes \epsilon)F = 1$$

(a cochain) does not change the representation category up to equivalence. In the present case, the twist transforms ϕ into $\phi_F = 1$, that is, into an ordinary Hopf algebra isomorphic over formal power series to $U_q(\mathfrak{g})$. Note that in rational conformal field theory the tensor product of representations appears as a finite-dimensional commutative associative algebra (the Verlinde algebra) with integer structure constants N_k^{ij} (this comes from the operator-product expansion of primary fields in the theory). This is because one has more precisely a truncated representation category corresponding to q a root of unity, and because we are identifying equivalent representations (so N_k^{ij} are the multiplicity in the decomposition of a tensor product of two representations). However, if one wants to know the tensor product decomposition more fully, not just its isomorphism class, this is given in a choice of bases by recoupling matrices. Computation in terms of these shows that the actual tensor product is neither commutative nor associative, but of the form above at least in the case of the WZW model.

Hopf algebra theory typically extends to the quasi-Hopf case. For example, given a quasi-Hopf algebra H there is a quantum double $D(H)$ at least in the finite-dimensional case, due to the author. An example is to take $H = C(G)$ and ϕ a 3-cocycle on G in the usual sense

$$\begin{aligned}\phi(y, z, w)\phi(x, yz, w)\phi(x, y, z) \\ = \phi(x, y, zw)\phi(xy, z, w)\end{aligned}$$

on elements of G and $\phi(x, 1, y) = 1$. Then $(C(G), \phi)$ can be viewed as a quasi-Hopf algebra. Its double $D^\phi(G)$ is generated by $C(G)$ as a sub-quasi-Hopf algebra and by elements of G with

$$\begin{aligned}x \cdot y &= yx \sum_s \delta_s \chi(y, x)(s), \quad \delta_s \cdot x = x\delta_{x s x^{-1}} \\ \Delta x &= \sum_{ab=s} \frac{\phi(x, x^{-1}ax, x^{-1}bx)\phi(a, b, x)}{\phi(a, x, x^{-1}bx)} \\ &\quad \times x\delta_a \otimes x\delta_b\end{aligned}$$

in terms of a basis $\{\delta_s\}$ of $C(G)$, the product of G on the right, and

$$\chi(x, y)(s) = \frac{\phi(x, y, y^{-1}x^{-1}sxy)\phi(s, x, y)}{\phi(x, x^{-1}sx, y)}$$

a 2-cocycle on G with values in $C(G)$ (the algebra is a cocycle semidirect product). There is a quasitriangular structure $\mathcal{R} = \sum \delta_x \otimes x$. This quasi-Hopf algebra first appeared in discrete topological quantum field theory related to orbifolds in the work of Dijkgraaf, Pasquier, and Roche.

There are further generalizations in the same spirit and which are linked to conformal field theories of more general type; for example, weak (quasi-) Hopf algebras in which $\Delta 1 \neq 1 \otimes 1$ but is a projector. These have been related to quantum groupoids.

Finally, we mention some applications of twisting outside of the original context. First of all, we are not limited to starting with $U(\mathfrak{g})$: starting with any Hopf algebra or quasi-Hopf algebra H we can similarly twist it to another one H_F with the same algebra as H and $\Delta_F, \mathcal{R}_F, \phi_F$ given by conjugation as above. The representation category remains unchanged up to equivalence, so in some sense the twisted object is equivalent. Moreover, if we start with a Hopf algebra H and ask F to be a 2-cocycle in the sense

$$F_{12}(\Delta \otimes \text{id})(F)(\text{id} \otimes \Delta)(F^{-1})F_{23}^{-1} = 1$$

then H_F will remain a Hopf algebra. It has conjugated antipode (see Majid 1995)

$$S_F(a) = U(Sa)U^{-1}, \quad U = \cdot(\text{id} \otimes S)(F)$$

Many Hopf algebras are twists of more standard ones, for example, the multiparameter quantum groups tend to be twists of the standard $U_q(\mathfrak{g})$. Likewise, “triangular” Hopf algebras (where $\mathcal{R}_{21}\mathcal{R}=1$) tend to be twists of classical group or enveloping algebras.

A second application of twists is an approach to quantization. Although it can be applied to H itself, this is more interesting if we think of H as a background quantum group and ask to quantize objects covariant under H . For the sake of discussion, we start with H an ordinary Hopf algebra. We twist this to H_F and denote by \mathcal{T} the equivalence functor from representations of H to representations of H_F . This functor acts as the identity on all objects and all morphisms, but comes with nontrivial isomorphisms $c_{V,W}: \mathcal{T}(V) \otimes \mathcal{T}(W) \rightarrow \mathcal{T}(V \otimes W)$ for any two objects, compatible with bracketing (see Majid 1995). Given any algebraic construction covariant under H , we simply apply the functor \mathcal{T} to all aspects of the construction and obtain an equivalent H_F -covariant construction. As an example, if A is an H -covariant algebra, then applying \mathcal{T} to its product we have $\mathcal{T}(\cdot): \mathcal{T}(A \otimes A) \rightarrow \mathcal{T}(A)$. Using $c_{A,A}$ we obtain a map

$$\begin{aligned} \bullet: \mathcal{T}(A) \otimes \mathcal{T}(A) &\rightarrow \mathcal{T}(A) \\ a \bullet b &= \cdot(F^{-1} \triangleright (a \otimes b)) \end{aligned}$$

in terms of the product in A . Thus, we have a new algebra A_F built on the same vector space as A but with a modified \bullet product. This is called a “covariant twist” of an algebra and should not be confused with the Drinfeld twist above. It is due to the author in the early 1990s. If F is a 2-cocycle, then A_F remains associative. The transmutation construction mentioned in the section “Self-dual quantum groups” or the passage from \mathbb{R}_q^4 to $\mathbb{R}_q^{1,3}$ are examples in quantum group theory. Other examples include the standard Moyal product on \mathbb{R}^n , also called noncommutative spacetime $[x_\mu, x_\nu] = i\theta_{\mu\nu}$ by string theorists (see Bicrossproduct Hopf Algebras and Noncommutative Spacetime).

If we do not demand that F is a cocycle, then the algebra A_F is still associative but in the target category, which means

$$(a \bullet b) \bullet c = (\bullet(\bullet))\Phi_{A,A,A}((a \otimes b) \otimes c)$$

Such objects are called “quasialgebras.” It may still be that $\Phi_{A,A,A}$ happens to be trivial (ϕ_F happens to act trivially) so that A_F remains associative. This turns out frequently to be the case and many quantizations in physics, including $C_q[G]$ but not limited to q -examples, can be obtained in this way. It means that although they are associative there is a hidden nonassociativity which can surface in other constructions involving Φ . The physical application here is with $H = U(\mathfrak{g})$ a classical enveloping algebra, A functions on a classical manifold on which \mathfrak{g} acts, and a cochain F . In general the resulting quasialgebra will not be associative but rather a quantization of a “quasi-Poisson manifold” obeying

$$\{a, \{b, c\}\} + \text{cyclic} = 2\tilde{n}(a \otimes b \otimes c)$$

Here \tilde{n} is the trivector field for the action of the lowest order part of ϕ_F and the (quasi)Poisson bivector is the leading-order part of $F_{21}F^{-1}$. As mentioned, there are many cases where \tilde{n} (and the action of the rest of ϕ_F) happens to be trivial.

Finally, let us give a discrete example using such quantum group methods. We consider $H = C(G)$ and $F \in C(G \times G)$ a cochain. Twisting by this gives $H_F = (C(G), \phi_F)$ a quasi-Hopf algebra where

$$\phi_F(x, y, z) = \frac{F(y, z)F((x, yz))}{F(xy, z)F(x, y)}$$

We take $A = \mathbb{C}G$ the group algebra. The action of $C(G)$ on it is the diagonal one. The modified algebra A_F therefore has product

$$x \bullet y = F^{-1}(x, y)xy$$

in terms of the product in G , and will be a quasialgebra if F is not a cocycle. For example, let

$G = (\mathbb{Z}_2)^3$ which we write additively (so elements are 3-vectors with values in \mathbb{Z}_2) and take

$$F(x, y) = (-1)^{\sum_{i < j} x_i y_j + y_1 x_2 x_3 + x_1 y_2 x_3 + x_1 x_2 y_3}$$

then,

$$\phi_F(x, y, z) = (-1)^{x \cdot (y \times z)}$$

Moreover, $A_F = O$, the octonions (Albuquerque and Majid 1999). So these are a nonassociative quantization of the classical discrete space $(\mathbb{Z}_2)^3$. We see that they are in fact associative up to sign and with sign +1 when the corresponding 3-vectors are linearly independent.

Noncommutative Geometry

In this article, we have frequently encountered the view of quantum groups and other noncommutative algebras as by definition the coordinate algebras on “noncommutative spaces.” However, the “quantum groups approach” to such noncommutative geometry that emerges has a somewhat different flavor from other approaches, as we discuss now.

In fact, the problem of geometry at such a level was mentioned already by Dirac in the 1920s and led to theorems of Gelfand and Naimark in the 1940s and 1950s whereby a noncommutative C^* -algebra should be viewed as a noncommutative topological space, and of Serre and Swan in the 1960s whereby a finitely generated projective module should be viewed as a vector bundle. Algebraic K -theory led to further refinement of this picture and particularly, in the 1980s, to A Connes’ formulation in terms of cyclic cohomology and “spectral triples” (see Noncommutative Geometry and the Standard Model; Noncommutative Tori, Yang–Mills and String Theory; Quantum Hall Effect; Hopf Algebra Structure of Renormalizable Quantum Field Theory; Path Integrals in Noncommutative Geometry). The quantum groups approach is less axiomatic, and consists of at least three disparate elements.

The first layer of the quantum groups approach is the theory of q -deformed groups and q -spaces on which they act, using braided category methods (such as braided linear spaces). The braided group additive law leads to partial derivatives and these define q -exterior algebras etc. This programme covered during the 1990s most of what is needed to q -deform physics in flat space at an algebraic level. Formulas here tend to be complex but controlled by R -matrices, and the correct R -matrix formulas can be found systematically by working

with braided algebra as explained in the section “Braided groups and quantum planes.” From a slightly different side, q -representation theory and the further theory of q -homogeneous spaces is intimately tied to a theory of q -special functions (such as the q -exponential function in the section “ q -Deformation enveloping algebras”) of interest in their own right (see q -Special Functions). The use of $*$ -algebras in some cases completable to C^* -algebras is a point of contact with other approaches to noncommutative geometry but problems emerge when one considers the braiding. As a result, the natural q -Poincaré (plus dilation) quantum group is not even a Hopf $*$ -algebra. Briefly, once one starts to braid the constructions, one may need to represent them with braided (not usual) Hilbert spaces and q -analysis.

The second layer of the quantum groups approach is based on “differential calculus” as a specification of an exterior algebra of differential forms or differential graded algebra (DGA). In general this is a wild problem but, as in classical geometry, the requirement of a quantum group covariance greatly narrows the possible calculi, although no longer to the point of uniqueness. The first examples of covariant calculi on the quantum group $C_q[SU_2]$ were found by Woronowicz (1989). The bicovariant one of these was cast in R -matrix form by Jurco while the first actual classification results on the moduli of irreducible calculi were obtained by the author (the bicovariant ones are essentially in correspondence with irreducible representations V , with left-invariant differentials forming a braided group of the form $B(V \otimes V^*)$). Probably the most interesting feature of this theory is that for all $C_q[G]$ the bicovariant q -calculus cannot be of classical dimensions. For example, for $C_q[SU_2]$ the smallest nontrivial calculus is four dimensional. The “extra dimension” is a biinvariant 1-form θ which has the property that $[\theta, a] = da$ for all $a \in C_q[SU_2]$ and which can be viewed as a spontaneously generated time (see Bicrossproduct Hopf Algebras and Noncommutative Spacetime). Quantum group methods also provide DGAs on finite groups, this time classified in the bicovariant case by nontrivial conjugacy classes. These therefore provide Lie structures on finite groups. One can go much further and define quantum principal bundles (with quantum groups as fiber) over general noncommutative algebras (Brzezinski and Majid 1993), associated bundles, frame bundles, and Riemannian geometry of the algebra (see Quantum Group Differentials, Bundles and Gauge Theory).

Again q -deformation provides key examples but the theory may then be applied to other situations.

For example, the permutation group S_3 has a natural connected calculus with dimensions $1 : 3 : 4 : 3 : 1$ (in other words the space has six points but each point has the local structure of a 4-manifold in some sense). It turns out to have a unique Levi-Civita type connection ∇ for its invariant metric, with constant curvature. The use of DGAs here is in common with other approaches (e.g., Connes 1994) and indeed bundles associated to quantum group principal bundles and suitable connections can be shown to be projective modules. The approaches diverge at the level of spectral triples, however, and the examples of “Dirac operators” that emerge from quantum group methods do not usually obey the required axioms.

A third established layer of the quantum groups approach is to trade some of the noncommutativity for nonassociativity, as in the dual version of Drinfeld’s construction, that is, $C_q[G]$ in terms of classical $C[G]$ as a (co)quasi-Hopf algebra. The general approach here is a quantization functor \mathcal{T} which provides all constructions but which will typically bring out the underlying nonassociative geometry even when the noncommutative covariant algebras of interest is associative. For example, applying the functor to the classical exterior algebra $\Omega(G)$ gives a bicovariant $\Omega(C_q[G])$ of classical dimensions but with nonassociative products (it is a supercoquasi-Hopf algebra). As before, one may then apply these quantum group methods to other algebras not related to q -deformation.

Beyond these are many recent developments, some of which are covered in other articles. Probably one of the most interesting frontiers, at the time of writing, is the exploration of links of both quantum groups and noncommutative geometry to number theory.

See also: Affine Quantum Groups; Axiomatic Approach to Topological Quantum Field Theory; Bicrossproduct Hopf Algebras and Noncommutative Spacetime; Braided and Modular Tensor Categories; Classical r -Matrices, Lie Bialgebras, and Poisson Lie Groups; Duality in Topological Quantum Field Theory; Eight Vertex and Hard Hexagon Models; Hopf Algebra Structure of Renormalizable Quantum Field Theory; The Jones Polynomial; Noncommutative Geometry and the Standard Model; Noncommutative Tori, Yang–Mills and String Theory; Path Integrals in Noncommutative

Geometry; q -Special Functions; Quantum Group Differentials, Bundles and Gauge Theory; Quantum Hall Effect; Symmetries in Quantum Field Theory of Lower Spacetime Dimensions; Topological Quantum Field Theory: Overview; von Neumann Algebras: Subfactor Theory; Yang–Baxter Equations.

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h-Pseudodifferential Operators and Applications

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From Classical Mechanics to Quantum Mechanics

The initial goal of semiclassical mechanics was to explore the correspondence principle, due to N Bohr in 1923, which states that one should recover the classical mechanics from the quantum mechanics as the Planck constant h tends to zero. So we start with a very brief presentation of these two theories.

Classical Mechanics

We start (with the Hamiltonian formalism) from a C^∞ function p on $\mathbb{R}^{2n} : (x, \xi) \mapsto p(x, \xi)$, which describes the motion of the system under consideration and is called the Hamiltonian. The variable x corresponds, in the simplest case, to the position and ξ to the momentum of one particle. The evolution is then described, starting at time 0 of a given point (y, η) , by the so-called Hamiltonian equations

$$\begin{aligned} \frac{dx_j}{dt} &= (\partial p / \partial \xi_j)(x(t), \xi(t)), \quad \text{for } j = 1, \dots, n \\ \frac{d\xi_j}{dt} &= -(\partial p / \partial x_j)(x(t), \xi(t)), \quad \text{for } j = 1, \dots, n \end{aligned} \quad [1]$$

The classical trajectories are then defined as the integral curves of a vector field defined on \mathbb{R}^{2n} called the Hamiltonian vector field associated with p and defined by $H_p = (\partial p / \partial \xi, -\partial p / \partial x)$. All these definitions are more generally relevant in the framework of symplectic geometry on a symplectic manifold M (but we choose, for simplicity, to explain the theory on \mathbb{R}^{2n}), which can be seen as the cotangent vector bundle $T^*\mathbb{R}^n$, and is the “local” model of the general situation. This space is equipped naturally with a symplectic structure defined by giving at each point a nondegenerate 2-form, which is here $\sigma := \sum_j d\xi_j \wedge dx_j$. This 2-form permits us to associate canonically to a 1-form on $T^*\mathbb{R}^n$ a vector field on $T^*\mathbb{R}^n$. In this correspondence, if p is a function on $T^*\mathbb{R}^n$, H_p is associated with the differential dp .

In this article, we consider the example of the Hamiltonian $p(x, \xi) = \xi^2 + V(x)$, also called the Schrödinger Hamiltonian, as the guiding example. More specifically, the case of the harmonic oscillator, where V is given by $V(x) = \sum_{j=1}^n \mu_j x_j^2$ (with $\mu_j > 0$), is the most significant, which is the natural approximation of a potential near its minimum, when nondegenerate.

In the framework of the classical mechanics, the main questions could be:

- Are the trajectories bounded?
- Are there periodic trajectories?
- Is one trajectory dense in its energy surface?
- Is the energy surface compact?

The solution of these questions could be very difficult. Let us just mention the trivial fact that, if $p^{-1}(\lambda)$ is compact for some λ , then, by the conservation of energy law

$$p(x(t), y(t)) = p(y, \eta) \quad [2]$$

the whole trajectory starting of one point (y, η) remains in the bounded set $\{p^{-1}(p(y, \eta))\}$ in \mathbb{R}^{2n} . This is in particular the case for the harmonic oscillator.

Quantum Mechanics

The quantum theory was born dynamics-wise around 1920. It is structurally related to the classical mechanics in a way that we shall describe very briefly. In quantum mechanics, our basic object will be a (possibly nonbounded) self-adjoint operator defined on a dense subspace of a Hilbert space \mathcal{H} . In order to simplify the presentation, we shall always take $\mathcal{H} = L^2(\mathbb{R}^n)$.

This operator can be associated with p by using the techniques of quantization. We choose here to present a procedure, called the Weyl quantization procedure (which was already known in 1928), which under suitable assumptions on p and its derivatives, will be defined for $u \in \mathcal{S}(\mathbb{R}^n)$ by

$$\begin{aligned} p^w(x, hD_x, h)u(x) &= (2\pi h)^{-n} \iint \exp\left(\frac{i}{h}(x-y) \cdot \xi\right) \\ &\quad \times p\left(\frac{x+y}{2}, \xi, h\right)u(y) dy d\xi \end{aligned} \quad [3]$$

The operator $p^w(x, hD_x, h)$ is called an h -pseudodifferential operator of Weyl symbol p . One can also write $\text{Op}_h^w(p)$ in order to emphasize that it is the operator associated to p by the Weyl quantization. Here h is a parameter which plays the role of the Planck constant.

Of course, one has to give a sense to these integrals and this is the object of the theory of the oscillatory integrals. If $p=1$, we observe that, by Plancherel's formula,

$$\begin{aligned} u(x) &= (2\pi h)^{-n} \iint \exp\left(\frac{i}{h}(x-y) \cdot \xi\right) \\ &\quad \times u(y) dy d\xi \end{aligned} \quad [4]$$

the associated operator is nothing but the identity operator. A way to rewrite any h -differential operator $\sum_{|\alpha| \leq m} a_\alpha(x) (hD_x)^\alpha$ as an h -pseudodifferential operator is to apply it on both sides to [4]. In particular, we observe that if the symbol is $p(x, \xi) = \xi^2 + V(x)$, then the operator associated with p by the h -Weyl quantization is the Schrödinger operator $-h^2\Delta + V$. Other interesting examples appear naturally in solid state physics. Let us, for example, mention the Harper operator H (or almost-Mathieu; see Helffer and Sjöstrand (1989) and references therein), whose symbol is the map $(x, \xi) \mapsto \cos \xi + \cos x$, and which can also be defined, for $u \in L^2(\mathbb{R})$, by

$$(Hu)(x) = \frac{1}{2}(u(x+h) + u(x-h)) + \cos x u(x)$$

We shall later recall how to relate the properties of p and those of the associated operator. More precisely, we shall describe under which conditions on p the operator $p^w(x, hD_x; h)$ is semibounded, symmetric, essentially self-adjoint, compact, with compact resolvent, trace class, Hilbert-Schmidt (see Robert (1987) for an extensive presentation). But before looking at a more general situation, let us consider the case of the Schrödinger operator $S_h = -h^2\Delta + V(x)$. If V is (say, continuous) bounded from below, S_h , which is *a priori* defined on $\mathcal{S}(\mathbb{R}^n)$ as a differential operator, admits a unique self-adjoint extension on $L^2(\mathbb{R}^n)$. We are first interested in the nature of the spectrum. If $V(x) \rightarrow +\infty$ as $|x| \rightarrow \infty$, one can show that S_h , more precisely its self-adjoint realization, has compact resolvent and its spectrum consists of a sequence of eigenvalues tending to ∞ . We are next interested in the asymptotic behavior of these eigenvalues.

In the case of the harmonic operator, corresponding to the potential

$$V(x) = \sum_{j=1}^n \mu_j x_j^2 \quad (\text{with } \mu_j > 0)$$

the criterion of compact resolvent is satisfied and the spectrum is described as the set of

$$\lambda_\alpha(h) = \sum_{j=1}^n \sqrt{\mu_j} (2\alpha_j + 1)h$$

for $\alpha \in \mathbb{N}^n$.

In this case we also have a complete description of the normalized associated eigenfunctions which are constructed recursively starting from the first eigenfunction corresponding to $\lambda_0(h) = \sum_j \sqrt{\mu_j} h$:

$$\phi_0(x; h) = \left(\prod_{j=1}^n \left(\frac{\sqrt{\mu_j}}{\pi h} \right)^{1/4} \right) \cdot \exp \left(-\frac{1}{2h} \sum_j \sqrt{\mu_j} x_j^2 \right) \quad [5]$$

The eigenfunction ϕ_0 is strictly positive and decays exponentially. Moreover (and here we enter in the semiclassical world), the local decay in a fixed closed set avoiding $\{0\}$ (which is measured by its L^2 -norm) is exponentially small as $h \rightarrow 0$. In particular, this says that the eigenfunction lives asymptotically in the set $\{V(x) \leq \lambda(h)\}$. This last set can also be understood as the projection by the map $(x, \xi) \mapsto x$ of the energy surface, which is classically attached to the eigenvalue $\lambda(h)$, that is, $\{(x, \xi) \in \mathbb{R}^{2n} \mid p(x, \xi) = \lambda(h)\}$. This is a typical semiclassical statement, which will be true in full generality.

From Quantum Mechanics to Classical Mechanics: Semiclassical Mechanics

Before describing the mathematical tools involved in the exploration of the correspondence principle, let us describe a few results which are typical in the semiclassical context. They concern Weyl's asymptotics and the localization of the eigenfunctions.

Weyl's asymptotics We start with the case of the Schrödinger operator S_h , but we emphasize that the h -pseudodifferential techniques are not limited to this situation.

We assume that V is a C^∞ -function on \mathbb{R}^n which is semibounded and satisfies

$$\inf V < \lim_{|x| \rightarrow \infty} V(x)$$

The Weyl theorem (which is a basic theorem in spectral theory) implies that the essential spectrum is contained in

$$\left[\lim_{|x| \rightarrow \infty} V(x), +\infty \right]$$

It is also clear that the spectrum is contained in $[\inf V, +\infty]$. In the interval

$$I = \left[\inf V, \lim_{|x| \rightarrow \infty} V(x) \right]$$

the spectrum is discrete, that is, it has only isolated eigenvalues with finite multiplicity. For any E in I , it is consequently interesting to look at the counting function $N_h(E)$ of the eigenvalues contained in $[\inf V, E]$,

$$N_h(E) = \#\{\lambda_j(h); \lambda_j(h) \leq E\} \quad [6]$$

The main semiclassical result is then

Theorem 1 *With the previous assumptions, we have:*

$$\lim_{h \rightarrow 0} h^n N_h(E) = (2\pi)^{-n} \int_{V(x) \leq E} (E - V(x))^{n/2} dx$$

of an explicit description of the eigenfunctions. This is quite important to have a good description of the decay of the eigenfunctions (as $h \rightarrow 0$) outside the classically permitted region without having to know an explicit formula. Various approaches can be used.

The first one fits very well in the case of the Schrödinger operator (more generally to h -pseudodifferential operators with symbols admitting holomorphic extensions in the ξ variable) and gives exponential decay. This is based on the so-called Agmon estimates (developed in the semiclassical context by Helffer–Sjöstrand and Simon). We shall not say more about this approach, which is the starting point of the analysis of the tunneling (see Helffer (1988), Dimassi and Sjöstrand (1999), and Martinez (2002)).

The second one is an elementary application of the h -pseudodifferential formalism which will be described later and leads, for example, to the following statement. Let E in I and let $(\lambda(h_j), \phi_{(h_j)}(x))$ be a sequence of spectral pairs in $I \times L^2(\mathbb{R}^n)$, where $h_j \rightarrow 0$ as $j \rightarrow +\infty$, $\lambda(h_j) \rightarrow E$, and $x \mapsto \phi_{(h_j)}(x)$ is an L^2 -normalized eigenfunction associated with $\lambda(h_j)$. Let Ω be a relatively compact set in \mathbb{R}^n such that

$$V^{-1}([-\infty, E]) \cap \bar{\Omega} = \emptyset$$

Then, there exists, for all integer N , a constant $C_{N,\Omega}$ such that

$$\|\phi_{(h_j)}\|_{L^2(\Omega)} \leq C_{N,\Omega} \cdot h_j^N$$

A third one uses the notion of frequency set and will be discussed later (see also the book of Martinez (2002) for what can be done with the Fourier–Bros–Iagolnitzer transform as developed by J Sjöstrand).

Brief Introduction to the h -Pseudodifferential Calculus

For fixed h , the pseudodifferential calculus has a long story starting in its modern form in the 1960s. A rather achieved version of the calculus is presented in Hörmander (1984). We will emphasize here on the semiclassical aspect of the calculus, that is, on the dependence of the calculus on the parameter $h > 0$.

h -Pseudodifferential Calculus

Basic calculus: the class S^0 We shall mainly discuss the most simple one called the S^0 calculus. Let us first say that the S^0 calculus is sufficient once we have suitably (micro)-localized the problem (e.g., by the functional calculus). Note that it is also sufficient for the local analysis of many problems occurring on compact manifolds.

This class of symbols p is simply defined by the conditions:

$$|\partial_x^\alpha \partial_\xi^\beta p(x, \xi)| \leq C_{\alpha, \beta} \quad [7]$$

for all $(\alpha, \beta) \in \mathbb{N}^n \times \mathbb{N}^n$. The symbols can possibly be h -dependent. With this symbol, one can associate an h -pseudodifferential operator by [3]. This operator is a continuous operator on $\mathcal{S}(\mathbb{R}^n)$ but can also be defined by duality on $\mathcal{S}'(\mathbb{R}^n)$.

The first basic analytical result is the Calderon–Vaillancourt theorem (see Hörmander (1984)) establishing the L^2 -continuity. We also mention that if p is in $L^2(\mathbb{R}^{2n})$, the associated operator is Hilbert–Schmidt. One can also give conditions on p implying the trace-class property (replace the uniform control in [7] by a control in L^1).

The second important property is the existence of a calculus. If a is in S^0 and b is in S^0 then the composition $a^w(x, hD_x) \circ b^w(x, hD_x)$ of the two operators is a pseudodifferential operator associated with an h -dependent symbol c in S^0 :

$$a^w(x, hD_x) \circ b^w(x, hD_x) = c^w(x, hD_x; h)$$

We see here that we immediately meet symbols admitting expansions in powers of h , which we shall call regular symbols, in the sense that they admit expansions of the type

$$a(x, \xi; h) \sim \sum_j a_j(x, \xi) h^j$$

$$b(x, \xi; h) \sim \sum_j b_j(x, \xi) h^j$$

In this case the Weyl symbol c of the composition has a similar expansion:

$$c(x, \xi; h) \sim \left[\exp\left(\frac{ih}{2}(D_x \cdot D_\eta - D_y \cdot D_\xi)\right) \times (a(x, \xi; h) \cdot b(y, \eta; h)) \right]_{x=y; \xi=\eta}$$

The symbol a_0 is called the principal symbol. At the level of principal symbols, the rule is simply that the principal symbol of $a^w \circ b^w$ is the product of the principal symbols of a^w and b^w : $c_0 = a_0 \cdot b_0$. Another important property is the following correspondence between commutator of two operators and Poisson brackets. The principal symbol of the commutator $(1/h)(a^w \circ b^w - b^w \circ a^w)$ is $(1/i)\{a_0, b_0\}$, where $\{f, g\}$ is the Poisson bracket of f and g :

$$\begin{aligned} \{f, g\}(x, \xi) &= H_f g \\ &= \sum_j (\partial_{\xi_j} f \cdot \partial_{x_j} g - \partial_{x_j} f \cdot \partial_{\xi_j} g) \end{aligned}$$

Everything is proved if $m(x, \xi) = (p_0 + 1)$ is a scale function, if p_j and their derivatives are controlled by $(p_0 + 1)$:

$$(H3) \quad |\partial_x^\alpha \partial_\xi^\beta p_j(x, \xi)| \leq C_{\alpha, \beta, j} (p_0 + 1) \phi(x, \xi)^{-j-|\alpha|} \times \Phi(x, \xi)^{-j-|\beta|}$$

for all $(\alpha, \beta) \in \mathbb{N}^n \times \mathbb{N}^n$, and if there is a suitable control of the family $(N \in \mathbb{N})$ of symbols

$$\left(\frac{\phi \Phi}{(p_0 + 1)h} \right)^{(N+1)} \left(p - \sum_{j=0}^N p_j h^j \right)$$

Under these assumptions, the main result is that P is, for h small enough, essentially self-adjoint. This means that the operator which was initially defined on $S(\mathbb{R}^n)$ by the pseudodifferential operator with symbol p admits a unique self-adjoint extension.

The Functional Calculus

It is well known by the spectral theorem for a self-adjoint operator P that a functional calculus exists for Borel functions. What is important here is to find a class of functions (actually essentially C_0^∞) such that $f(P)$ is a pseudodifferential operator in the same class as P with simple rules of computation for the principal symbol.

We are starting from the general formula (see Dimassi and Sjöstrand (1999))

$$f(P) = -\pi^{-1} \lim_{\epsilon \rightarrow 0^+} \int \int_{|\operatorname{Im} z| \geq \epsilon} \frac{\partial \tilde{f}}{\partial \bar{z}}(x, y) (z - P)^{-1} dx dy$$

which is true for any self-adjoint operator and any f in $C_0^\infty(\mathbb{R})$. Here the function $(x, y) \mapsto \tilde{f}(x, y)$ (note that $z = x + iy$) is a compactly supported, almost analytic extension of f to \mathbb{C} . This means that $\tilde{f} = f$ on \mathbb{R} and that for any $N \in \mathbb{N}$ there exists a constant C_N such that

$$\left| \frac{\partial \tilde{f}}{\partial \bar{z}}(z) \right| \leq C_N |\operatorname{Im} z|^N$$

The main result due to Helffer–Robert (see also Dimassi and Sjöstrand (1999) and references therein) is that, for P an h -regular pseudodifferential operator satisfying (H0)–(H3) and f in $C_0^\infty(\mathbb{R})$, the operator $f(P)$ is an h -pseudodifferential operator, whose Weyl symbol $p_f(x, \xi; h)$ admits a formal expansion in powers of h :

$$p_f(x, \xi; h) \sim \sum_{j \geq 0} h^j p_{f,j}(x, \xi)$$

with

$$p_{f,0} = f(p_0)$$

$$p_{f,1} = p_1 \cdot f'(p_0)$$

$$p_{f,j} = \sum_{k=1}^{2j-1} (-1)^k (k!)^{-1} d_{j,k} f^{(k)}(p_0), \quad \forall j \geq 2$$

where the $d_{j,k}$ are universal polynomial functions of the symbols $\partial_x^\alpha \partial_\xi^\beta p_\ell$, with $|\alpha| + |\beta| + \ell \leq j$.

The main point in the proof is that we can construct, for $\operatorname{Im} z \neq 0$, a parametrix (= approximate inverse) for $(P - z)$ with a nice control as $\operatorname{Im} z \rightarrow 0$. The constants controlling the estimates on the symbols are exploding as $\operatorname{Im} z \rightarrow 0$ but the choice of the almost analytic extension of f absorbs any negative power of $|\operatorname{Im} z|$.

As a consequence, we get that if, for some interval I and some $\epsilon_0 > 0$,

$$(H4) \quad p_0^{-1}(I + [-\epsilon_0, \epsilon_0]) \text{ is compact}$$

then the spectrum is, for h small enough, discrete in I .

In particular, we get that, if $p_0(x, \xi) \rightarrow +\infty$ as $|x| + |\xi| \rightarrow +\infty$, then the spectrum of P_h is discrete (P_h has compact resolvent). Under the assumption (H4), we get more precisely the following theorem.

Theorem 3 *Let P be an h -regular pseudodifferential operator satisfying (H0)–(H4), with $I = [E_1, E_2]$, then, for any g in $C_0^\infty([E_1, E_2])$, we have the following expansion in powers of h :*

$$\operatorname{tr}[g(P(h))] \sim h^{-n} \sum_{j \geq 0} h^j T_j(g), \quad \text{as } h \rightarrow 0$$

where $g \mapsto T_j(g)$ are distributions in $\mathcal{D}'([E_1, E_2])$. In particular, we have

$$T_0(g) = (2\pi)^{-n} \iint g(p_0(x, \xi)) dx d\xi$$

$$T_1(g) = (2\pi)^{-n} \iint g'(p_0(x, \xi)) p_1(x, \xi) dx d\xi$$

This theorem is just obtained by integration of the preceding one, because in these cases the trace of a trace-class pseudo-differential operator $\operatorname{Op}^w(a)$ is given by the integral of the symbol a over $\mathbb{R}^{2n} = \mathbb{R}_x^n \times \mathbb{R}_\xi^n$. According to [3], the distribution kernel is given by the oscillatory integral:

$$K(x, y; h) = (2\pi h)^{-n} \int_{\mathbb{R}^n} \exp\left(\frac{i}{h}(x - y) \cdot \xi\right) \times a\left(\frac{x + y}{2}, \xi; h\right) d\xi \quad [8]$$

Fourier Integral Operators

We have already given in [8] the distribution kernel of an h -pseudodifferential operator. It appears useful to generalize this point of view by considering more generally objects defined similarly as

$$K(x, y; h) = (2\pi h)^{-r} \int_{\mathbb{R}^N} \exp\left(\frac{i}{h} \phi(x, y, \theta)\right) a(x, y, \theta; h) d\theta$$

There are a lot of examples entering in this framework. The representation of the metaplectic group in $L^2(\mathbb{R}^n)$ appears to be in this class, with the specificity that the phase is quadratic (Guillemin and Sternberg (1977)). A quite elementary case corresponds to the case when $N=0$ and $\phi(x, y) = x \cdot y$. No θ variable is present and so no integration appears with respect to θ . When $a=1$, this defines essentially the Fourier transform. Under suitable conditions on ϕ and a , one can show that the associated operators are continuous on $S(\mathbb{R}^n)$ (this is, of course, the case for the Fourier transform). This was done by Asada and Fujiwara, who transpose the theory developed by Hörmander (1971) in this context, and we should also mention the older (but more formal) work by Maslov (1972) (see also Leray (1981)). We actually do not need it in the semiclassical context because the case when the amplitude is with compact support is sufficient.

The basic object is first to look, thinking of the stationary-phase theorem, which gives the main contribution as $h \rightarrow 0$ in this "formal integral" (see Stationary Phase Approximation), at the critical set \mathcal{C}_ϕ :

$$\mathcal{C}_\phi = \{(x, y, \theta) \in \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^N \mid (\partial_\theta \phi)(x, y, \theta) = 0\}$$

In the case of a pseudodifferential operator, we find that it is included in $\{x=y\}$. Then we associate the canonical object, which is a Lagrangian submanifold called Λ_ϕ and defined as

$$\Lambda_\phi = \{(x, \xi, y, \eta) \mid \exists \theta \text{ s.t. } \xi = \nabla_x \phi(x, y, \theta), \\ \eta = -\nabla_y \phi(x, y, \theta), \nabla_\theta \phi(x, y, \theta) = 0\}$$

The assumptions on ϕ (which are omitted here) are given in order to get that Λ_ϕ is a regular manifold at least on the support of a . The associated operators are called Fourier integral operators (FIOs). L. Hörmander (1971, 1984) has developed a general and more intrinsic machinery but with a homogeneity condition on the phase which is irrelevant in the semiclassical context. This theory permits also the reduction to normal forms for Hamiltonians in continuation of what can be done in classical mechanics.

Quantum Evolution

We just sketch how one approximates the operator $\exp(-itP/h)$ by an FIO. The formal construction is probably rather old (Maslov 1972, Fedoryuk and Maslov 1981) but the rigorous approach with estimates of the remainders was first considered by J Chazarain with rather strong assumptions. It has been later realized that we need only a local approximation of this operator and everything becomes easier.

The first approach followed by Helffer–Robert (see Robert (1987)) is to localize in energy, within the functional calculus associated to the operator P . If I is an interval and χ is with compact support in I , it appears to be easier to approximate $\exp(-itP/h)\chi(P)$ when P satisfies (H4) in a neighborhood of I .

We do not need any more assumptions at ∞ and the composition by $\chi(P)$ localizes the construction.

Although this construction is simple because we remain within a functional calculus which involves only functions of P , it is not always sufficient to localize in energy. We have then to localize through more general h -pseudodifferential operators and consider $\exp(-itP/h)a^w(x, hD_x)$, where a is a symbol with compact support. We shall quickly develop the first approach. The result is that one can approximate $U_\chi(t) := \chi(P) \exp(-itP/h)$ by a Fourier integral operator of the form

$$K_\chi(t, x, y; h) = (2\pi h)^{-n} \int^{\text{osc}} \exp\left(-\frac{i}{h}(S(t, x, \eta) - y \cdot \eta)\right) \\ \times d_\chi(t, x, \eta; h) d\eta$$

with $d_\chi \sim \sum_j d_{\chi, j} h^j$, in order to have

$$\left\| \chi(P) \exp\left(-\frac{itP}{h}\right) - K_\chi(t) \right\|_{\mathcal{L}(L^2)} = \mathcal{O}(h^\infty)$$

Writing that $U_\chi(t)$ is a solution of $(hD_t + P)U_\chi = 0$, $(U_\chi)(0) = \chi(P)$, and expanding in powers of h , one gets a sequence of equations permitting to determine recursively the symbols. The first one was analyzed in [12] and reads, in the case when $P = -h^2 \Delta + V$:

$$(\partial_t S)(t, x, \eta) + |\nabla_x S(t, x, \eta)|^2 + V(x) = 0$$

with the initial condition $S(0, x, \eta) = x \cdot \eta$.

This has been solved for t small enough. The other equations are called transport equations. The first one is, for $a(t, x, \eta) = d_{\chi, 0}(t, x, \eta)$,

$$\partial_t a + (\partial_\xi p_0)(x, \partial_x S(t, x, \eta)) \cdot \partial_x a + ca = f$$

with initial condition $a(0, x, \eta) = \chi(p_0(x, \eta))$.

This type of equation is easily solved by integration along the integral curves of the vector field $\partial_t + (\partial_\xi p_0)(x, \partial_x S(t, x, \eta)) \cdot \partial_x$.

The Poisson Relation

We start from the harmonic oscillator

$$H(h) = \frac{1}{2} \left(-h^2 \frac{d^2}{dx^2} + x^2 \right)$$

Its spectrum is given by $(n + 1/2)h$ ($n \geq 0$). Its symbol is $a_0(x, \xi) = (1/2)(\xi^2 + x^2)$ and the corresponding flow, for any strictly positive level E , is periodic with primitive period 2π . The quantity we are interested in is

$$S_b^\chi(t) := \sum_{j \in \mathbb{N}} \chi((j + \frac{1}{2})h) \exp(-it(j + \frac{1}{2}))$$

Using the classical Poisson relation,

$$\sum_{k \in \mathbb{Z}} \hat{f}(k) \exp(ikx) = (2\pi) \cdot \sum_{k \in \mathbb{Z}} f(x + 2k\pi)$$

one shows rather easily that the frequency set of S_χ is

$$\text{FS}(S_b^\chi) = \{(2k\pi, \tau) | \tau > 0, \\ \tau \in \text{supp } \chi, k \in \mathbb{Z}\} \cup (\mathbb{R} \times \{0\})$$

This admits the following generalization, initiated in this context by Chazarain.

Theorem 7 *Let P satisfy (H0)–(H4). Let χ be a function with compact support in I and let $t \mapsto f_\chi(t; h)$ be the family of distributions defined by*

$$f_\chi(t; h) = \text{tr} \left(\exp \left(-\frac{itP}{h} \right) \chi(P) \right)$$

Then $\text{FS}(f_\chi)$ is contained in

$$\{(t, \tau) | \tau \in \text{supp } (\chi) \text{ and } \exists (x, \xi) \text{ s.t.} \\ p_0(x, \xi) = \tau, \phi^t(x, \xi) = (x, \xi)\}$$

According to the definition, we have to study

$$\int \exp \left(-\frac{it\tau}{h} \right) \theta(t) f_\chi(t; h) dt$$

This takes the form

$$\int c(t, x, \eta) \exp \frac{i}{h} (-t\tau + S(t, x, \eta) - x\eta) dt dx d\eta$$

and can be analyzed by a nonstationary-phase theorem, in order to determine for which value of τ the quantity is $\mathcal{O}(h^\infty)$.

Gutzwiller's Formula

The Gutzwiller formula was established formally by Gutzwiller (1971). It then appears in the context of high-energy spectral asymptotics in contributions of Colin de Verdière, Chazarain, and Duistermaat

and Guillemin (see Duistermaat and Guillemin (1975), Hörmander (1984), Guillemin and Sternberg (1977); see also Semi-Classical Spectra and Closed Orbits and Quantum Ergodicity and Mixing of Eigenfunctions). In the semiclassical context, the simplest statement (cf. Chazarain, Helffer–Robert, Guillemin–Uribe, Meinrencken, Paul–Uribe, Dozias, Combescure–Ralston–Robert – see Robert (1987), Rauch and Simon (1997), Dimassi and Sjöstrand (1999), and in the recent article by Combescure *et al.* (1999) for techniques involving coherent states) can be presented in the following way. For a noncritical E , we introduce the energy surface $W_E = \{w \in T^*\mathbb{R}^n | p_0(w) = E\}$. Let $P(h)$ an h -pseudodifferential operator satisfying (H0)–(H4), with $I = \{E\}$. We also assume that

(Cl) The restriction of the flow $\phi_{p_0}^t$ to W_E is clean. (A flow ϕ^t , associated with a C^∞ -vector field X on a manifold W , is called clean if the two following properties are satisfied:

- the set $\Gamma = \{(t, w) \in \mathbb{R} \times W | \phi^t(w) = w\}$ is a submanifold of $\mathbb{R} \times W$;
- in each point $\gamma = (t, w)$ of Γ , the tangent space to Γ is given by $T_\gamma \Gamma = \{(\tau, v) \in \mathbb{R} \times T_w W | \tau X(w) + (D\phi^t)(w) \cdot v = v\}$.

Then there exists a sequence of distributions $\gamma_k \in \mathcal{D}'(\mathbb{R})$, such that, for all $\phi \in \mathcal{S}(\mathbb{R})$ with compactly supported Fourier transform, we have the asymptotic expansion in powers of h :

$$\sum_{\lambda_j(h) \in [E - \epsilon_0/2, E + \epsilon_0/2]} \phi(h^{-1}(\lambda_j(h) - E)) \\ \sim \sum_{j=0}^{\infty} \gamma_j(\hat{\phi}) h^{-n+1+j} \quad [13]$$

Moreover, the supports of the distributions are contained in the set of the periods of the periodic trajectories of the flow contained in W_E .

Actually, the proof gives more information on the structure of the different distributions. Let us just write the formula for γ_0 :

$$\gamma_0 = (\pi)^{-n/2} \left(\frac{d}{d\lambda} \int_{p(x, \xi) \leq \lambda} dx d\xi \right)_{\lambda=E} \delta_0$$

where δ_0 is the Dirac measure at 0.

Clustering of Eigenvalues

We shall mention one typical result due to Chazarain–Helffer–Robert in this context, but inspired by previous results obtained for the Laplacian on compact manifolds (see Semi-Classical Spectra and Closed Orbits, Quantum Ergodicity and Mixing of Eigenfunctions and references therein, including Chazarain, Duistermaat–Guillemin, and Colin de Verdière).

most sophisticated theorems on the counting functions (including boundaries, singularities,...) but is only written for specialists.

See also: Normal Forms and Semiclassical Approximation; Quantum Ergodicity and Mixing of Eigenfunctions; Resonances; Schrödinger Operators; Semiclassical Spectra and Closed Orbits; Stability of Matter; Stationary Phase Approximation.

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Hubbard Model

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Definitions

The Hubbard model is a standard theoretical model for strongly interacting electrons in a solid. It is a minimum model which takes into account both quantum many-body effects and strong nonlinear interaction between electrons. Here we review rigorous results on the Hubbard model, placing main emphasis on magnetic properties of the ground states.

Let the lattice Λ be a finite set whose elements $x, y, \dots \in \Lambda$ are called sites. Physically speaking, each site corresponds to an atomic site in a crystal. The Hubbard model is based on the simplest tight-binding description of electrons (Figure 1), where a single state is associated with each site.

For each $x \in \Lambda$ and $\sigma \in \{\uparrow, \downarrow\}$, we define the creation and the annihilation operators $c_{x,\sigma}^\dagger$ and $c_{x,\sigma}$, respectively, for an electron at site x with

spin σ . (A^\dagger is the adjoint or the Hermitian conjugate of A .) These operators satisfy the canonical anti-commutation relations

$$\begin{aligned} \{c_{x,\sigma}^\dagger, c_{y,\tau}\} &= \delta_{x,y} \delta_{\sigma,\tau} \\ \{c_{x,\sigma}^\dagger, c_{y,\tau}^\dagger\} &= \{c_{x,\sigma}, c_{y,\tau}\} = 0 \end{aligned} \quad [1]$$

for any $x, y \in \Lambda$ and $\sigma, \tau = \uparrow, \downarrow$, where $\{A, B\} = AB + BA$. The number operator is defined by

$$n_{x,\sigma} = c_{x,\sigma}^\dagger c_{x,\sigma} \quad [2]$$

which has eigenvalues 0 and 1.

The Hilbert space of the model is constructed as follows. Let Φ_{vac} be a normalized vector state which satisfies $c_{x,\sigma} \Phi_{\text{vac}} = 0$ for any $x \in \Lambda$ and $\sigma = \uparrow, \downarrow$. Physically, Φ_{vac} corresponds to a state where there are no electrons in the system. For arbitrary subsets $\Lambda_\uparrow, \Lambda_\downarrow \subset \Lambda$, we define

$$\Phi_{\Lambda_\uparrow, \Lambda_\downarrow} = \left(\prod_{x \in \Lambda_\uparrow} c_{x,\uparrow}^\dagger \right) \left(\prod_{x \in \Lambda_\downarrow} c_{x,\downarrow}^\dagger \right) \Phi_{\text{vac}} \quad [3]$$

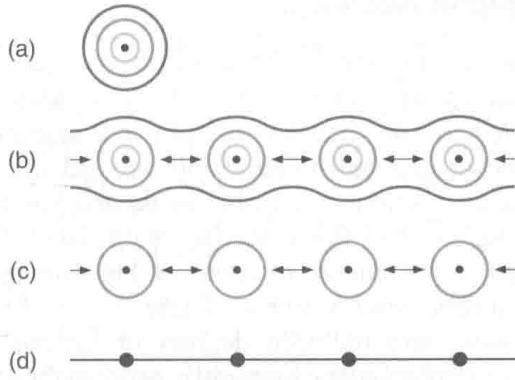


Figure 1 A highly schematic figure which explains the philosophy of tight-binding description. (a) A single atom which has multiple electrons in different orbits. (b) When atoms come together to form a solid, electrons in the black orbits become itinerant, while those in the light gray orbits are still localized at the original atomic sites. Electrons in the gray orbits are mostly localized around the atomic sites, but tunnel to nearby gray orbits with nonnegligible probabilities. (c) We only consider electrons in the gray orbits, which are expected to play essential roles in determining various aspects of low-energy physics of the system. (d) If the gray orbit is nondegenerate, we get a lattice model in which electrons live on lattice sites and hop from one site to another. In a simplified treatment of a metal, the black and the gray orbits correspond to the 4s and the 3d bands, respectively.

in which sites in Λ_\uparrow are occupied by up-spin electrons and sites in Λ_\downarrow by down-spin electrons. We fix the electron number N_e , which is an integer satisfying $0 < N_e \leq 2|\Lambda|$. (We denote by $|S|$ the number of elements in a set S .) The Hilbert space for the system with N_e electrons is spanned by the basis states [3] with all subsets Λ_\uparrow and Λ_\downarrow such that $|\Lambda_\uparrow| + |\Lambda_\downarrow| = N_e$.

We define total spin operators $\hat{S}_{\text{tot}} = (\hat{S}_{\text{tot}}^{(1)}, \hat{S}_{\text{tot}}^{(2)}, \hat{S}_{\text{tot}}^{(3)})$ by

$$\hat{S}_{\text{tot}}^{(\alpha)} = \frac{1}{2} \sum_{\substack{x \in \Lambda \\ \sigma, \tau = \uparrow, \downarrow}} c_{x, \sigma}^\dagger (p^{(\alpha)})_{\sigma, \tau} c_{x, \tau} \quad [4]$$

for $\alpha = 1, 2$, and 3 . Here $p^{(\alpha)}$ are the Pauli matrices

$$\begin{aligned} p^{(1)} &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, & p^{(2)} &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ p^{(3)} &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{aligned} \quad [5]$$

The operators \hat{S}_{tot} are the generators of global $\text{SU}(2)$ rotations of the spin space. As usual, we denote the eigenvalue of $(\hat{S}_{\text{tot}})^2$ as $S_{\text{tot}}(S_{\text{tot}} + 1)$. The maximum possible value of S_{tot} is $S_{\text{max}} = N_e/2$ when $N_e \leq |\Lambda|$, and $S_{\text{max}} = |\Lambda| - (N_e/2)$ when $N_e \geq |\Lambda|$.

The most general Hamiltonian of the Hubbard model is

$$H = - \sum_{\substack{x, y \in \Lambda \\ \sigma = \uparrow, \downarrow}} t_{x, y} c_{x, \sigma}^\dagger c_{y, \sigma} + \sum_{x \in \Lambda} U_x n_{x, \uparrow} n_{x, \downarrow} \quad [6]$$

Here the first term describes quantum-mechanical motion of electrons which hop around the lattice according to the amplitude $t_{x, y} = t_{y, x} \in \mathbb{R}$. Usually, $t_{x, y}$ is nonnegligible only when the two sites x and y are close to each other. The second term represents nonlinear interaction between electrons. There is an increase in energy by $U_x \in \mathbb{R}$ when the site x is occupied by both up-spin electron and down-spin electron. We usually set $U_x > 0$ to mimic (screened) Coulomb interaction between electrons.

* The Hamiltonian H commutes with the total spin operator $\hat{S}_{\text{tot}}^{(\alpha)}$ for $\alpha = 1, 2$, and 3 . One can thus investigate simultaneous eigenstates of $(\hat{S}_{\text{tot}})^2$ and H . For S_{tot} in the allowed range, we denote by $E_{\text{min}}(S_{\text{tot}})$ the lowest possible energy among the states which satisfy $(\hat{S}_{\text{tot}})^2 \Phi = S_{\text{tot}}(S_{\text{tot}} + 1)\Phi$.

Wave-Particle Dualism in the Hubbard Model

It is illuminating to examine the eigenstates of the Hamiltonian [6] for the following two special cases.

First suppose that one has $U_x = 0$ for all $x \in \Lambda$, that is, the model has no interactions. For $i = 1, 2, \dots, |\Lambda|$, let $\psi^{(i)} = (\psi_x^{(i)})_{x \in \Lambda} \in \mathbb{C}^\Lambda$ be the single-electron eigenstate, which is the solution of the Schrödinger equation

$$- \sum_{y \in \Lambda} t_{x, y} \psi_y^{(i)} = \epsilon_i \psi_x^{(i)} \quad \text{for any } x \in \Lambda \quad [7]$$

We order the energy eigenvalues as $\epsilon_i \leq \epsilon_{i+1}$. By defining the corresponding creation operator by $a_{i, \sigma}^\dagger = \sum_{x \in \Lambda} \psi_x^{(i)} c_{x, \sigma}^\dagger$, we see that, for any subsets $I_\uparrow, I_\downarrow \in \{1, 2, \dots, |\Lambda|\}$ such that $|I_\uparrow| + |I_\downarrow| = N_e$, the state

$$\Psi_{I_\uparrow, I_\downarrow} = \left(\prod_{i \in I_\uparrow} a_{i, \uparrow}^\dagger \right) \left(\prod_{i \in I_\downarrow} a_{i, \downarrow}^\dagger \right) \Phi_{\text{vac}} \quad [8]$$

is an eigenstate of H (with $U_x = 0$) with the eigenvalue $E = \sum_{i \in I_\uparrow} \epsilon_i + \sum_{i \in I_\downarrow} \epsilon_i$. The ground states are obtained by choosing I_\uparrow, I_\downarrow which minimize E . In particular, when N_e is even and the single-electron eigenenergies ϵ_i are nondegenerate, the ground state is unique and written as

$$\Phi_{\text{GS}} = \left(\prod_{i=1}^{N_e/2} a_{i, \uparrow}^\dagger a_{i, \downarrow}^\dagger \right) \Phi_{\text{vac}} \quad [9]$$

The fact that this ground state has the minimum possible spin $S_{\text{tot}} = 0$ is known as Pauli paramagnetism.

We have seen that the Hamiltonian H with $U_x = 0$ can be diagonalized by using single-electron

eigenstates $\psi^{(i)}$. When $(t_{x,y})$ has a translation invariance, each $\psi^{(i)}$ behaves as a “wave.” We can say that the noninteracting models can be understood in terms of the wave picture of electrons.

Next suppose that $t_{x,y}=0$ for all $x,y \in \Lambda$, that is, the electrons do not hop. Then the Hamiltonian [6] is readily diagonalized in terms of the basis state [3], where the corresponding eigenvalue is simply $E = \sum_{x \in \Lambda} U_x$. In this case, the model is best understood in the particle picture of electrons.

We thus see that the wave-particle dualism manifests itself in the Hubbard model in an essential manner. When both the first and the second terms in the Hamiltonian [6] are present, there takes place a “competition” between wave-like nature and particle-like nature of electrons. The competition generates rich nontrivial phenomena including antiferromagnetism, ferromagnetism, metal-insulator transition, and (probably) superconductivity. To investigate these phenomena is a major motivation in the study of the Hubbard model.

One-Dimensional Model

The Hubbard model defined on a simple one-dimensional lattice is easier to study. But it does not exhibit truly nontrivial behavior as the following classical theorem of Lieb and Mattis suggests.

Theorem 1 Consider a Hubbard model on a one-dimensional lattice $\Lambda = \{1, 2, \dots, N\}$ with open boundary conditions. We assume that $t_{x,y} \neq 0$ if $|x - y| = 1$, and $t_{x,y} = 0$ if $|x - y| > 1$. $t_{x,x} \in \mathbb{R}$ and $U_x \in \mathbb{R}$ are arbitrary. Then one has $E_{\min}(S_{\text{tot}}) < E_{\min}(S_{\text{tot}} + 1)$ for any $S_{\text{tot}} = 0, 1, \dots, S_{\text{max}} - 1$ (or $S_{\text{tot}} = 1/2, 3/2, \dots, S_{\text{max}} - 1/2$).

As a consequence, one finds that the ground states always have $S_{\text{tot}} = 0$ (or $S_{\text{tot}} = 1/2$) as in the noninteracting models.

The translation invariant model with $t_{x,y} = t$ if $|x - y| = 1$, $t_{x,y} = 0$ if $|x - y| \neq 1$, and $U_x = U$ can be solved by using the Bethe ansatz, as was first shown by Lieb and Wu. It was found that the model is insulating for all $U > 0$, and there is no metal-insulator transition. (A metal-insulator transition is expected to take place in higher dimensions.) Earlier works on the Bethe ansatz were based on the assumption that the Bethe ansatz equation gives the true ground states. Recently, the existence and the uniqueness of the Bethe ansatz solution for the ground state of a finite system was proved by Goldbaum.

Half-Filled Systems

The system in which the electron number N_e is identical to the number of sites $|\Lambda|$ is said to be half-filled. Many (but not all) physical systems can be modeled as a half-filled Hubbard model.

Based on a heuristic perturbation theory, low-energy properties of half-filled models with large U are expected to be similar to those of Heisenberg antiferromagnetic spin systems. There is no electrical conduction, and the spin degrees of freedom may show antiferromagnetic long-range order in the ground states.

This expectation is partly justified by the following theorem due to Lieb. A Hubbard model is said to be bipartite if the lattice Λ can be decomposed into a disjoint union of two sublattices as $\Lambda = A \cup B$ (with $A \cap B = \emptyset$), and it holds that $t_{x,y} = 0$ whenever $x, y \in A$ or $x, y \in B$. In other words, only hopping between different sublattices is allowed.

Theorem 2 Consider a bipartite Hubbard model. We assume $|\Lambda|$ is even, and the whole Λ is connected through nonvanishing $t_{x,y}$. We also assume $U_x = U > 0$ for any $x \in \Lambda$. Then the ground states of the model are nondegenerate apart from the trivial spin degeneracy, and have total spin $S_{\text{tot}} = ||A| - |B||/2$. It also holds that $E_{\min}(S_{\text{tot}}) < E_{\min}(S_{\text{tot}} + 1)$ for any $S_{\text{tot}} \geq ||A| - |B||/2$.

The theorem implies that, as far as the total spin is concerned, the half-filled Hubbard model behaves exactly as the Heisenberg antiferromagnet. But the existence of antiferromagnetic ordering has not been proved in any version of the Hubbard model.

To see another implication of Theorem 2, take the so-called CuO lattice in Figure 2. Here the A and B sublattices consist of black and white sites, respectively. One has $|A| = |\Lambda|/3$ and $|B| = 2|\Lambda|/3$. Then the theorem implies that the ground state of the corresponding Hubbard model has total spin

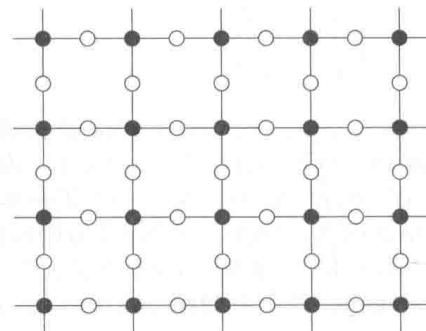


Figure 2 An example (the so-called CuO lattice) of a bipartite lattice in which the numbers of sites in two sublattices are different. Lieb's theorem implies that the half-filled Hubbard model defined on this lattice exhibits ferrimagnetism.

$S_{\text{tot}} = ||A| - |B||/2 = |\Lambda|/6$. Since the total spin magnetic moment of the system is proportional to the number of sites $|\Lambda|$, we conclude that the model exhibits ferrimagnetism, a weaker version of ferromagnetism.

Another interesting result for the half-filled models is the following uniform density theorem by Lieb, Loss, and McCann.

Theorem 3 *Consider a bipartite Hubbard model. $t_{x,y} \in \mathbb{R}$, $U_x \in \mathbb{R}$ are arbitrary. Suppose that the ground states are n -fold degenerate, and let $\Phi_{\text{GS}}^{(i)}$ ($i=1, \dots, n$) be mutually orthogonal normalized ground states. Define the correlation function by $\rho(x, y) = n^{-1} \sum_{i=1}^n \langle \Phi_{\text{GS}}^{(i)}, (c_{x,\uparrow}^\dagger c_{y,\uparrow} + c_{x,\downarrow}^\dagger c_{y,\downarrow}) \Phi_{\text{GS}}^{(i)} \rangle$. ($\langle \cdot, \cdot \rangle$ is the inner product.) Then for any $x, y \in A$ or $x, y \in B$, one has $\rho(x, y) = \delta_{x,y}$.*

It is interesting that the density $\rho(x, x)$ in the ground state is always unity though the hopping matrix and interactions can be highly nonuniform.

Ferromagnetism

Ferromagnetism is an interesting phenomenon in which the majority of the spins in the system align in the same direction. One of the original motivations to study the Hubbard model was to understand the origin of ferromagnetism in an idealized situation. Let us recall that neither the hopping term nor the interaction term in the Hamiltonian [6] favors ferromagnetism (or any other magnetic order). One must deal with the interplay between the two terms to have ferromagnetism. Here we review three rigorous examples of saturated ferromagnetism in the Hubbard model. Saturated ferromagnetism is the strongest form of ferromagnetism where the ground state has $S_{\text{tot}} = S_{\text{max}}$.

The first example is due to Nagaoka and Thouless.

Theorem 4 *Take an arbitrary finite lattice Λ , and let $N_e = |\Lambda| - 1$. Assume that $t_{x,y} \leq 0$ for any $x \neq y$, and let $U_x \rightarrow \infty$ for all $x \in \Lambda$. (Taking the limit $U_x \rightarrow \infty$ is equivalent to inhibiting x from being occupied by two electrons.) Then among the ground states of the model, there exist states with total spin $S_{\text{tot}} = S_{\text{max}} (= N_e/2)$. If the system further satisfies the connectivity condition (see below), then the ground states have $S_{\text{tot}} = S_{\text{max}} (= N_e/2)$ and are nondegenerate apart from the trivial spin degeneracy.*

The connectivity condition is a simple condition which holds in most of the lattices in two or higher dimensions, including the square lattice, the triangular lattice, or the cubic lattice. To be precise the condition requires that “by starting from any

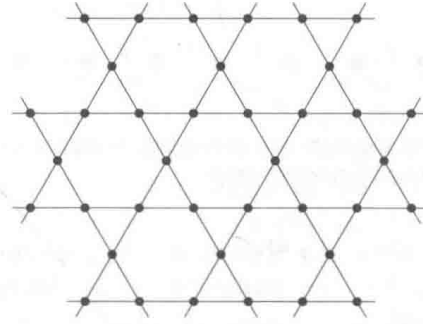


Figure 3 The Hubbard model on the kagomé lattice is a typical example which exhibits flat-band ferromagnetism.

electron configuration on the lattice and by moving around the hole along nonvanishing $t_{x,y}$, one can get any other electron configuration.”

The requirements that $U_x \rightarrow \infty$ and $N_e = |\Lambda| - 1$ are indeed rather pathological. We still do not know if the ferromagnetism extends to more realistic situations. Heuristic studies indicate that the issue is highly delicate.

A completely different class of rigorous examples of ferromagnetism was found by Mielke. Take, for example, the kagomé lattice of Figure 3, and define a Hubbard model by setting $t_{x,y} = t < 0$ when x and y are neighboring, $t_{x,y} = 0$ otherwise, and $U_x = U \geq 0$ for any $x \in \Lambda$. Then the corresponding single-electron Schrödinger equation [7] has a peculiar feature that its ground states are $\{(|\Lambda|/3) + 1\}$ -fold degenerate. This huge degeneracy corresponds to the fact that the lowest-energy band of the model is completely dispersionless (or flat).

Theorem 5 *Consider the Hubbard model on the kagomé lattice with $N_e = (|\Lambda|/3) + 1$. For any $U > 0$, the ground states have $S_{\text{tot}} = S_{\text{max}} (= N_e/2)$ and are nondegenerate apart from the trivial spin degeneracy.*

There are similar examples in higher dimensions. Ferromagnetism observed in these models is called flat-band ferromagnetism.

The above examples of ferromagnetism have either singular interaction ($U_x \rightarrow \infty$) or singular dispersion relation (highly degenerate single-electron ground states). Tasaki found a class of Hubbard models which are free from such singularities, and exhibit ferromagnetism.

For simplicity, we concentrate on the simplest model in one dimension. There are similar examples in higher dimensions. Take the one-dimensional lattice $\Lambda = \{1, 2, \dots, N\}$ with N sites (where N is an even integer), and impose a periodic boundary condition by identifying the site $N + 1$ with the site 1. The hopping matrix is defined by setting $t_{x,x+1} = t_{x+1,x} = -t'$ for any $x \in \Lambda$, $t_{x,x+2} = t_{x+2,x} = -t$ for even x , $t_{x,x+2} = t_{x+2,x} = s$ for odd x , and $t_{x,y} = 0$

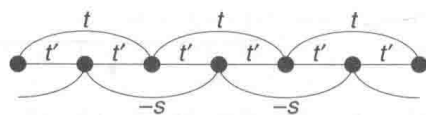


Figure 4 An example of nonsingular Hubbard model which exhibits saturated ferromagnetism.

otherwise. Here $t > 0$ and $s > 0$ are independent parameters, but the parameter t' is determined as $t' = \sqrt{2}(t + s)$.

As can be seen from Figure 4, electrons are allowed to hop to next-nearest neighbors. Thus, Theorem 1 does not apply. The single-electron ground states are not degenerate unless $s = 0$. We set $U_x = U > 0$ for any $x \in \Lambda$, and fix the electron number as $N_e = N/2$. In terms of filling factor, this corresponds to the quarter filling.

Theorem 6 Suppose that the two dimensionless parameters t/s and U/s are sufficiently large. Then the ground states have $S_{\text{tot}} = S_{\text{max}} (= N/4)$ and are nondegenerate apart from the trivial spin degeneracy.

The theorem is valid, for example, when $t/s \geq 4.5$ if $U/s = 50$, and $t/s \geq 2.6$ if $U/s = 100$. It is crucial that the statement of the theorem is valid only when the interaction U is sufficiently large. In the same model, it is also proved that low-lying excitation above the ground state has a normal dispersion relation of a spin-wave excitation.

We would like to point out that one can learn more details about the Hubbard model and further

rigorous results from the review articles (Lieb 1995, Tasaki 1998a, Tasaki 1998b). One can also find references for most of the results discussed here in these review articles, especially in Lieb (1995).

As for the latest results which are not included in the above reviews, see recent publications, for example, Lieb and Wu (2003), Tasaki (2003), and Goldbaum (2005), and references therein.

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Hydrodynamic Equations see Interacting Particle Systems and Hydrodynamic Equations

Hyperbolic Billiards

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Introduction

Billiards are a class of dynamical systems with appealingly simple description. A point particle moves with constant velocity in a box of arbitrary dimension (the billiard table) and reflects elastically from the boundary (the component of velocity

perpendicular to the boundary is reversed and the parallel component is preserved). Mathematically, it is a class of Hamiltonian systems with collisions defined by symplectic maps on the boundary of the phase space. The billiard dynamics defines a one-parameter group of maps Φ^t of the phase space which preserve the Lebesgue measure, and are in general only measurable due to discontinuities. The boundaries of the box are made up of pieces, concave, convex, and flat. Discontinuities occur at the orbits tangent to concave pieces of the boundary of the box. The orbits hitting two adjacent pieces ("corners") cannot be naturally

continued, which is another source of discontinuities. These singularities are not too severe so that the flow has well-defined Lyapunov exponents and Pesin structural theory is applicable (Katok and Strelcyn 1986). A billiard system is called hyperbolic if it has nonzero Lyapunov exponents on a subset of positive Lebesgue measure, and completely hyperbolic if all of its Lyapunov exponents are nonzero almost everywhere, except for one zero exponent in the direction of the flow.

Billiards in smooth strictly convex domains have no singularities, but no such examples are known to be hyperbolic.

In general, billiards exhibit mixed behavior just like other Hamiltonian systems; there are invariant tori intertwined with "chaotic sea." In hyperbolic billiards, stable behavior is excluded by the choice of the pieces in the boundary of the box, arbitrary concave pieces and special convex ones, and their particular placement. Thus, hyperbolicity is achieved by design, as in optical instruments.

It was established by Turaev and Rom-Kedar (1998) that complete hyperbolicity may be lost under generic singular perturbation of the billiard system to a smooth Hamiltonian system.

Hyperbolicity is the universal mechanism for random behavior in deterministic dynamical systems. Under suitable additional assumptions, it leads to ergodicity, mixing, K -property, Bernoulli property, decay of correlations, central-limit theorem, and other stochastic properties. Hyperbolic billiards provide a natural class of examples for which these properties were studied. In this article we restrict ourselves to hyperbolicity itself.

The most prominent example of a hyperbolic billiard is the gas of hard spheres. This way of looking at the system was developed in the groundbreaking papers of Sinai (see Chernov and Sinai (1987) for an exhaustive list of references). The collection of papers (Szász 2000) contains more up-to-date information. Another source on hyperbolic billiards is the book by Chernov and Markarian (2005). The books by Kozlov and Treschev (1990), and by Tabachnikov (1995) provide broad surveys of billiards from different perspectives.

Jacobi Fields and Monotonicity

The key to understanding hyperbolicity in billiards lies in two essentially equivalent descriptions of infinitesimal families of trajectories. The basic notion is that of a Jacobi field along a billiard trajectory. Let $\gamma(t, u)$ be a family of billiard trajectories, where t is time and u is a parameter,

$|u| < \epsilon$. A Jacobi field along $\gamma(t, 0)$ is defined by $J(t) = \partial\gamma/\partial u|_{u=0}$.

Jacobi fields form a finite-dimensional vector space which can be identified with the tangent to the phase space at points along the trajectory. They contain the same information as the derivatives of the billiard flow $D\Phi^t$. In particular, the Lyapunov exponents are the exponential rates of growth of Jacobi fields.

Jacobi fields split naturally into parallel and perpendicular components to the trajectory, each of them a Jacobi field in its own right. The parallel Jacobi field carries the zero Lyapunov exponent. In the rest we discuss only the perpendicular Jacobi fields. Between collisions the Jacobi fields satisfy the differential equation $J'' = 0$, hence $J(t) = J(0) + tJ'(0)$. At a collision a Jacobi field undergoes a change by the map

$$\begin{aligned} J(t_c^+) &= \mathcal{R}J(t_c^-) \\ J'(t_c^+) &= \mathcal{R}J'(t_c^-) + \mathcal{P}^* \mathcal{K} \mathcal{P} J(t_c^+) \end{aligned} \quad [1]$$

where $J(t_c^-)$ and $J(t_c^+)$ are Jacobi fields immediately before and after collision, \mathcal{K} is the shape operator of the piece of the boundary ($\mathcal{K} = \nabla n$, n is the inside unit normal to the boundary), and \mathcal{P} is the projection along the velocity vector from the hyperplane perpendicular to the orbit to the hyperplane tangent to the boundary. Finally, \mathcal{R} is the orthogonal reflection in the hyperplane tangent to the boundary.

Perpendicular Jacobi fields at a point of a trajectory can be identified with a subspace of the tangent to the phase space, the subspace perpendicular to the phase trajectory. To measure the growth/decay of Jacobi fields, we introduce a quadratic form on the tangent spaces, or equivalently on Jacobi fields, $\mathcal{Q}(J, J') = \langle J, J' \rangle$. Evaluation of \mathcal{Q} on a Jacobi field is a function of time $\mathcal{Q}(t)$. Between collisions we have $\mathcal{Q}(t_2) \geq \mathcal{Q}(t_1)$ for $t_2 \geq t_1$ (monotonicity). By [1] the monotonicity at the collisions, that is, $\mathcal{Q}(t_c^+) \geq \mathcal{Q}(t_c^-)$ is equivalent to the positive semidefiniteness of the shape operator $\mathcal{K} \geq 0$, it holds for concave pieces of the boundary. If $\mathcal{K} > 0$ at a point of collision with the boundary, then for $(J, J') \neq (0, 0)$, we have $\mathcal{Q}(t_2) > \mathcal{Q}(t_1)$ (strict monotonicity), assuming that the collision occurred between time t_1 and t_2 .

In billiards with concave pieces of the boundary, where $\mathcal{K} \geq 0, \mathcal{K} \neq 0$, strict monotonicity may still occur after sufficiently many reflections (eventual strict monotonicity, or ESM). Such billiards are called semidispersing, and the gas of hard spheres is an example.

The role of monotonicity is revealed in the following:

Theorem 1 (Wojtkowski 1991). *If a system is eventually strictly monotone (ESM), except on a set of orbits of zero measure, then it is completely hyperbolic.*

The theorem applies to billiard systems. It can be generalized and applied to other systems, not even Hamiltonian (see Wojtkowski (2001) for precise formulations, references and the history of this idea).

The difficulty in applying the above theorem to the gas of hard spheres lies in the gap between monotonicity and strict monotonicity. There are many orbits on which strict monotonicity is never attained (parabolic orbits). Establishing that the family of parabolic orbits has measure zero (or better yet codimension 2) is a formidable task. It was brought to conclusion in the work of Simányi (2002).

Wave Fronts and Monotonicity

There is a geometric formulation of monotonicity (which historically preceded the one given above). Let us consider a local wave front, that is, a local hypersurface $W(0)$ perpendicular to a trajectory $\gamma(t)$ at $t=0$. Let us consider further all billiard trajectories perpendicular to $W(0)$. The points on these trajectories at time t form a local hypersurface $W(t)$ perpendicular again to the trajectory (warning: at exceptional moments of time the wave front $W(t)$ may be singular). Infinitesimally wave fronts are described by the shape operator $U = \nabla n$, where n is the unit normal field. U is a symmetric operator on the hyperplane tangent to the wave front (and perpendicular to the trajectory $\gamma(t)$). The evolution of infinitesimal wave fronts is described by the formulas

$$\begin{aligned} U(t) &= (tI + U(0)^{-1})^{-1} && \text{without collisions} \\ U(t_c^+) &= \mathcal{R}U(t_c^-)\mathcal{R} + \mathcal{P}^*\mathcal{K}\mathcal{P} && \text{at a collision} \end{aligned} \quad [2]$$

It follows that between collisions a wave front that is initially convex (i.e., diverging, or $U > 0$) will stay convex. Moreover, any wave front after a sufficiently long run without collisions will become convex (after which the normal curvatures of the wave front will be decaying). The second part of [2] shows that after a reflection in a strictly concave boundary a convex wave front becomes strictly convex (and its normal curvatures increase). These properties are equivalent to (strict) monotonicity as formulated above. Indeed, in the language of Jacobi

fields an infinitesimal wave front represents a linear subspace in the space of perpendicular Jacobi fields, that is, the tangent space. (Furthermore, it is a Lagrangian subspace with respect to the standard symplectic form.) We can follow individual Jacobi fields or whole subspaces of them. It explains the parallel of [1] and [2]. The form \mathcal{Q} allows the introduction of positive and negative Jacobi fields and positive and negative Lagrangian subspaces. An infinitesimal convex wave front represents a positive Lagrangian subspace. Monotonicity is equivalent to the property that a positive Lagrangian subspace stays positive under the dynamics (it may appear that there is a loss of information in formulas [2] compared to [1], but actually they are equivalent due to the symplectic nature of the dynamics (Wojtkowski 2001).

Design of Hyperbolic Billiards

In view of [2] it seems that a convex piece in the boundary ($K < 0$) excludes monotonicity. There are two ways around this obstacle. First, we could change the quadratic form \mathcal{Q} at the convex boundary. Second, we can treat convex pieces as “black boxes” and look only at incoming and outgoing trajectories. Although the second strategy seems more restrictive, all the examples constructed to date fit the black box scenario, and we will present it in more detail.

To understand this approach, let us consider a billiard table with flat pieces of the boundary and exactly one convex piece. A trajectory in such a billiard experiences visits to the convex piece separated by arbitrary long sequences of reflections in flat pieces, which do not affect the geometry of a wave front at all. Hence, whatever is the geometry of a wave front emerging from the curved piece it will become convex and very flat by the time it comes back to the curved piece of the boundary again. Hence, it follows, at least heuristically, that we must study the complete passage through the convex piece of the boundary, regarding its effect on convex, and especially flat, wave fronts.

Important difference between convex and concave pieces is that a trajectory has usually several consecutive reflections in the same convex piece; moreover, the number of such reflections is unbounded. A finite billiard trajectory is called “complete” if it contains reflections in one and the same piece of the boundary, and it is preceded and followed by reflections in other pieces.

Definition A complete trajectory is (strictly) z -monotone if for every nonzero Jacobi field the

value of the form Q (increases) does not decrease between the point at the distance z before the first reflection and the point at the distance z after the last reflection.

A complete trajectory is parabolic if there is a nonzero Jacobi field J such that J' vanishes before the first and after the last reflection.

In the language of wave fronts, a complete trajectory is z -monotone if every diverging wave front at a distance at least z from the first reflection becomes diverging after the last reflection at the distance z , or earlier.

It turns out that the only obstruction to monotonicity of complete trajectories is parabolicity. More precisely, if a complete trajectory is not parabolic then it is z -monotone for some $z > 0$.

It follows from Theorem 1 that we get a completely hyperbolic billiard if we put together curved pieces with no complete parabolic trajectories and some flat pieces, in such a way that for every two consecutive complete trajectories, being z_1 - and z_2 -monotone, respectively, the distance from the last reflection in the first trajectory to the first reflection in the second one is bigger than $z_1 + z_2$. Indeed, we can put together the midpoints of trajectories leaving one curved piece and hitting another one into the Poincaré section of the billiard flow and we obtain immediately ESM for the return map.

We can formulate somewhat informally two principles for the design of hyperbolic billiards.

1. *No parabolic trajectories* Convex pieces of the boundary cannot have complete parabolic trajectories.
2. *Separation* There must be enough separation (in space or in time through reflections in flat pieces) between strictly z -monotone trajectories according to the values of z .

All of the examples of hyperbolic billiards constructed up to now are designed according to these principles.

Hyperbolic Billiards in Dimension 2

Checking the absence of parabolic trajectories is nontrivial due to the unbounded number of reflections in complete trajectories close to tangency. It was accomplished so far only in integrable, or near integrable examples, with the exception of convex scattering pieces described in the following.

Billiards in dimension 2 are understood best. First of all, there is yet another way of describing infinitesimal families of nearby trajectories. Every

infinitesimal family of rays in the plane has a point of focusing (in linear approximation), possibly at infinity. This point of focusing contains the same information as the curvature of a wave front (it is the center of curvature, rather than curvature itself) and it has the advantage that it does not change between collisions. The focusing points before and after a reflection are related by the familiar mirror equation of the geometric optics:

$$-\frac{1}{f_0} + \frac{1}{f_1} = \frac{2}{d}$$

where f_0, f_1 are the signed distances of the points of focusing to the reflection point, $d = r \cos \theta$, r being the radius of curvature of the boundary piece ($r > 0$ for a strictly convex piece), and θ the angle of incidence. The mirror equation is just the two dimensional version of [2].

It is instructive to consider an arc of a circle. A billiard in a disk is integrable due to its rotational symmetry. Let J be a Jacobi field obtained by rotation of a trajectory. This family of trajectories ("the rotational family") is focused exactly in the middle between two consecutive reflections (that is where J vanishes). It follows further from the mirror equation that a parallel family of orbits is focused at a distance $d/2$ after the reflection, and any family focusing somewhere between the parallel family and the rotational family will focus at a distance somewhere between $d/2$ and d , not only after the first reflection, but also after arbitrary long sequence of reflections.

Hence, any complete trajectory in an arc of a circle is z -monotone, where $2z$ is the length of a single segment of the trajectory and strictly z' -monotone for any $z' > z$. Two arcs of a circle separated by parallel segments form the stadium of Bunimovich (1979).

Lazutkin (1973) showed that billiards in smooth strictly convex domains are near integrable near the boundary. Donnay (1991) applied Lazutkin's coordinates to establish that for an arbitrary strictly convex arc the situation near the boundary is similar to that in a circle, that is, complete trajectories near tangency are z -monotone, where z is of the order of the length of a single segment. In particular, no near tangent complete trajectory can be parabolic. Hence, this crucial calculation shows that if a strictly convex arc has no parabolic trajectories then any sufficiently small perturbation also has no parabolic trajectories. It follows further that any sufficiently small piece of a given strictly convex arc has no parabolic trajectories.

It turns out that in dimension 2, complete parabolic trajectories are also z -monotone for some

$z > 0$ (but clearly not strictly monotone) (Wojtkowski 2005). However, they are still an obstacle to complete hyperbolicity because in general nearby complete trajectories are z -monotone without a bound for the values of z , so that no separation of convex pieces is sufficient.

Integrability of the elliptic billiard allows one to establish strict monotonicity of trajectories in the semi-ellipse with endpoints on the longer axis, Wojtkowski 1986. Donnay (1991) showed that also the semi-ellipse with endpoints on the shorter axis has no parabolic trajectories provided that the eccentricity is less than $\sqrt{2}/2$. As the eccentricity goes to $\sqrt{2}/2$ the separation required to produce a hyperbolic billiard goes to infinity. Markarian *et al.* (1996) obtained explicitly the separation of the elliptic pieces needed for hyperbolicity, when the eccentricity is smaller than $\sqrt{2} - \sqrt{2}/2$.

It follows from the mirror equation that a trajectory with one reflection in a convex piece is always strictly z -monotone for $z > d$. Hence, if for any two consecutive reflections in convex pieces with respective values of d equal to d_1 and d_2 , the distance between reflections exceeds $d_1 + d_2$, then the billiard is completely hyperbolic. For one convex piece this condition, called convex scattering, turns out to be equivalent to $d^2 r/ds^2 < 0$, where s is the arc length (Wojtkowski 1986). This leads to examples of hyperbolic billiards with one convex piece of the boundary, like the domain bounded by the cardioid.

Also, any complete trajectory in a convex scattering piece is strictly z -monotone for z bigger than the maximum of the values of d for the first and the last segment of the trajectory. This allows to find easily the explicit separation of convex scattering pieces guaranteeing hyperbolicity.

Hyperbolic Billiards in Higher Dimensions

In higher dimensions, only two constructions of hyperbolic billiards with convex pieces in the boundary are known. The first construction by Bunimovich (1988), involves a piece of a sphere whose angular size, as seen from the center, does not exceed $\pi/2$ (Wojtkowski 1990, 2005, Bunimovich and Rehacek 1998). The second construction by Papenbrock (2000) uses two cylinders, at 90° with respect to each other to destroy integrability (Wojtkowski 2005). In both cases, the successful treatment is based on integrability of the billiard systems bounded by a sphere or a cylinder.

In both of these constructions, trajectories need to be cut into strictly monotone pieces of unbounded lengths. In the case of spherical caps, complete

trajectories are z -monotone with unbounded value of z and the geometry of the billiard table is used to separate them in time by sufficiently many reflections in flat pieces of the boundary (Wojtkowski 2005). In the case of cylinders, trajectories are cut by consecutive returns to a Poincaré section in the middle of the billiard table.

Soft Billiards

The same ideas of monotonicity and strict monotonicity are applicable to soft billiards, where specular reflections are replaced by scatterers in which the point particle is subjected to the action of a spherically symmetric potential. As in ordinary billiards, we compare the wave fronts along trajectories before entering and after leaving scatterers. Again, in the absence of parabolic trajectories sufficient separation of the scatterers produces a completely hyperbolic system.

The conditions on the potential that guarantee the absence of parabolic trajectories were obtained by Donnay and Liverani (1991) in the two-dimensional case and by Bálint and Tóth (2006) in higher dimensions. The complete integrability of the motion of a point particle in a spherically symmetric potential is crucial in the derivation of these conditions (Wojtkowski 2005).

See also: Billiards in Bounded Convex Domains; Ergodic Theory; Hamiltonian Systems: Stability and Instability Theory; Hyperbolic Dynamical Systems; Polygonal Billiards; Random Matrix Theory in Physics.

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Hyperbolic Dynamical Systems

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Introduction

Division of Smooth Dynamical Systems

Linear maps can be elliptic (complex diagonalizable with all eigenvalues on the unit circle), parabolic (all eigenvalues on the unit circle but some Jordan blocks of size at least 2), or hyperbolic (no eigenvalues on the unit circle), and for differentiable dynamical systems, that is, smooth maps or flows, one can roughly make an analogous subdivision (see Hasselblatt and Katok 2002, p. 100f). The linear maps not covered by these alternatives are those with some eigenvalues on the unit circle and others off it; the corresponding class of “partially hyperbolic” dynamical systems is usually considered in the context of hyperbolic dynamical systems with a view to studying phenomena wherein the hyperbolic behavior dominates. Thus, elliptic dynamical systems are more or less similar to isometries, with orbit separation constant or at most oscillatory but without persistent growth. KAM theory deals with elliptic systems, establishing that much of the ellipticity in an integrable Hamiltonian system persists under perturbation. Parabolic systems may have polynomial orbit separation produced by a local “shear” phenomenon; billiards in polygonal domains are an example of this. Hyperbolic dynamical systems are characterized by exponential divergence of

orbits. They are of interest because of the complexity of their orbit structure with respect to both topological and statistical behavior.

Specifically, the stretching (corresponding to eigenvalues outside the unit circle in the case of linear maps) combined with the folding necessitated by compactness of the phase space produces not only highly sensitive dependence of orbit asymptotics on initial conditions, but also a close intertwining of different behaviors. On the one hand, there is a dense set of periodic points, on the other hand, an abundance of dense orbits. While there are only finitely many periodic points of a given period, their number grows exponentially as a function of the period. The entropy of these systems is positive, which indicates that the overall complexity of the orbit structure grows exponentially as a function of the length of time for which it is being tracked. In effect, the behavior of orbits is so intricate as to be quasirandom, which makes it natural to use statistical methods to describe these systems.

History of Hyperbolic Dynamical Systems

One strand of the history of hyperbolic dynamical systems leads back to the question of the stability of the solar system and to Poincaré, in whose prize memoir on the three-body problem the possibility of “homoclinic tangles” first presented itself. For Poincaré, this was important because the resulting complexity demonstrates that this system is not integrable. We describe below how hyperbolic dynamics arises in this situation (see Figure 3).

Another strand emerged about a decade later with Hadamard's study of geodesic flows (free particle motion) on negatively curved surfaces. Hadamard noted that these exhibit the kind of sensitive dependence on initial conditions as well as the pseudorandom behavior that are central features of hyperbolic dynamics. This subject was developed much further after the advent of ergodic theory, with the Boltzmann ergodic hypothesis as an important motivation: work by numerous mathematicians, principally Hedlund and Hopf, showed that free particle motion on a negatively curved surface provides examples of ergodic mechanical systems. More than two decades later, in the 1960s, Anosov and Sinai overcame a fundamental technical hurdle and established that this is indeed the case in arbitrary dimension. This was done in the more general context of a class of dynamical systems known now as Anosov systems, which were axiomatically defined and systematically studied for the first time during this period of research in Moscow.

A greater class of dynamical systems exhibiting chaotic behavior was introduced by Smale in his seminal 1967 paper under the name of Axiom-A systems. This class includes the hyperbolic dynamics arising from homoclinic tangles, see Figure 3 (see Homoclinic Phenomena). Smale's motivation was his program of classifying dynamical systems under topological conjugacy, and the consequent search for structurally stable systems. Today, Axiom-A (and Anosov) systems are valued as idealized models of chaos: while the conditions defining Axiom A are too stringent to include many real-life examples, it is recognized that they have features shared in various forms by most chaotic systems. Here, we concentrate on the discrete-time context to keep notations lighter.

Partial hyperbolicity was introduced in the 1970s and has proved that a limited amount of hyperbolicity in a dynamical system can produce much of the global complexity (such as ergodicity or the presence of dense orbits) exhibited by hyperbolic systems, and can do so in a robust way. Here one imposes uniform conditions, but expansion and contraction are not assumed to occur in all directions. Stable ergodicity has been an important subject of research in the last decade.

Nonuniform hyperbolicity weakens hyperbolicity by allowing the contraction and expansion rates to be nonuniform. This was motivated by examples of systems with hyperbolicity where expansion or contraction can be arbitrarily weak or absent in places, such as the Hénon attractor, and by situations where hyperbolicity coexists with singularities, such as for (semi)dispersing billiards (see Hyperbolic Billiards).

With respect to both uniformly and nonuniformly hyperbolic systems, dimension theory has been a subject of much interest (computations and estimates of the fractal dimension of attractors and hyperbolic sets, which is deeply connected to dynamical properties of the system).

A different weakening of hyperbolicity, the presence of a dominated splitting, has been of interest from the a viewpoint to stability and classification of diffeomorphisms.

The study of hyperbolic dynamics has always had interactions with other sciences and other areas of mathematics. In the natural and social sciences, this is the study of chaotic motions of just about any kind. Examples of applications in related areas of mathematics are geometric rigidity (an interaction with differential geometry) and rigidity of group actions.

Uniformly Hyperbolic Dynamical Systems

Definitions

Let f be a smooth invertible map. A compact invariant set of f is said to be "hyperbolic" if at every point in this set, the tangent space splits into a direct sum of two subspaces E^u and E^s with the property that these subspaces are invariant under the differential df , that is, $df(x)E^u(x) = E^u(f(x))$, $df(x)E^s(x) = E^s(f(x))$, and that df expands vectors in E^u and contracts vectors in E^s , that is, there are constants $0 < \lambda < 1 < \mu, c > 0$ such that if $v \in E^s(x)$ for some x , then $\|df^n v\| \leq c\lambda^n \|v\|$ for $n = 1, 2, \dots$, and if $v \in E^u(x)$ for some x , then $\|df^{-n} v\| \leq c\mu^{-n} \|v\|$ for $n = 1, 2, \dots$.

If $E^u = \{0\}$ in the definition above, then the invariant set is made up of attracting fixed points or periodic orbits. Similarly, if $E^s = \{0\}$, then the orbits are repelling. If neither subspace is trivial, then the behavior is locally "saddle-like," that is to say, relative to the orbit of a point x , most nearby orbits diverge exponentially fast in both forward and backward time. This is why hyperbolicity is a mathematical notion of chaos.

An Anosov diffeomorphism is a smooth invertible map of a compact manifold with the property that the entire space is a hyperbolic set.

Axiom A, which is a larger class, focuses on the part of the system that is not transient. More precisely, a point x in the phase space is said to be "nonwandering" if every neighborhood U of x contains an orbit that returns to U . A map is said to satisfy Axiom A if its nonwandering set is hyperbolic and contains a dense set of periodic points.

Definitions in the continuous-time case are analogous: f above is replaced by the time- t -maps of the flow, and the tangent spaces now decompose into $E^u \oplus E^0 \oplus E^s$ where E^0 , which is one dimensional, represents the direction of the flow lines.

A geometric way of detecting (indeed, defining) hyperbolicity is via the cone criterion: at every point there is a cone that is mapped by the differential into the interior of the corresponding cone at the image point, and a “complementary” cone family behaves similarly for the inverse.

Many continuous structures associated with a hyperbolic dynamical system are, in fact, Hölder continuous. (For a function g on a metric space this is defined as the existence of $C, \alpha > 0$ such that $d(g(x), g(y)) \leq C d(x, y)^\alpha$ whenever x, y are sufficiently close to each other.) In the present article, almost every assertion of continuity could be replaced by one of Hölder continuity. This notion is natural in this context because $x_n \rightarrow y$ exponentially fast implies that $g(x_n) \rightarrow g(y)$ exponentially fast if g is Hölder continuous.

Structure and Properties

Stable and Unstable Manifolds, Local Product Structure

Anosov and Axiom-A systems are defined by the behavior of the differential. Corresponding to the linear structures left invariant by df are nonlinear structures, namely “stable manifolds” tangent to E^s and “unstable manifolds” tangent to E^u .

Thus, associated with an Anosov map are two families of invariant manifolds, each one of which fills up the entire phase space; they are sometimes called the stable and unstable “foliations.” The leaves of these foliations are transverse at each point, that is, they intersect at positive angles, forming a kind of (topological) coordinate system. The map f expands distances along the leaves of one of these foliations and contracts distances along the leaves of the other. For Axiom-A systems, one has a similar local product structure or “coordinate system” at each point in the nonwandering set, but the picture is local, and there are gaps: the stable and unstable leaves do not necessarily fill out open sets in the phase space.

There is much interest in determining the fractal dimension (box-counting or Hausdorff, say) of hyperbolic sets. So far the best dimension estimates have been made for stable slices, that is, for the intersection of a stable leaf with the hyperbolic set, and for unstable slices. Because the local coordinate systems describing the local product structure are

only known to be continuous, it is not known in general whether the sum of these stable and unstable dimensions gives the dimension of the hyperbolic set (we don’t even know whether all stable slices have the same fractal dimension). The problem is that an α -Hölder-continuous map can change dimensions by a factor of α or $1/\alpha$. But there is evidence to suggest that something like this “dimension product structure” may often be true – this has been established for a class of solenoids.

Transitivity and Spectral Decomposition

In addition to these local structures, Axiom-A systems have a global structure theorem known as “spectral decomposition.” It says that the nonwandering set of every Axiom-A map can be written as $X_1 \cup \dots \cup X_r$ where the X_i are disjoint closed invariant sets on which f is topologically transitive, that is, has a dense orbit. The X_i are called “basic sets.” Each X_i can be decomposed further into a finite union $\bigcup X_{i,j}$, where each $X_{i,j}$ is invariant and topologically mixing under some iterate of f . (Topological transitivity and mixing are irreducibility conditions; transitivity means that there is no proper open invariant subset, and topological mixing says that given two open sets, from some time onward the images of one will always intersect the other.) This decomposition is reminiscent of the corresponding result for finite-state Markov chains.

Stability

One of the reasons why hyperbolic sets are important is their “robustness”: they cannot be perturbed away. More precisely, let f be a map with a hyperbolic set Λ which is locally maximal, that is, it is the largest invariant set in some neighborhood U . Then for every map g that is C^1 -near f , the largest invariant set Λ' of g in U is again hyperbolic; moreover, f restricted to Λ is “topologically conjugate” to g restricted to Λ' . This is mathematical shorthand for saying that not only are the two sets Λ and Λ' topologically indistinguishable, but the orbit structure of f on Λ is indistinguishable from that of g on Λ' .

The phenomenon above brings us to the idea of “structural stability.” A map f is said to be structurally stable if every map g C^1 -near f is topologically conjugate to f (on the entire phase space). It turns out that a map is structurally stable if and only if it satisfies Axiom A and an additional condition called strong transversality.

Chains and Shadowing

We discuss next the idea of pseudo-orbits versus real orbits. Letting $d(\cdot, \cdot)$ be the metric, a sequence of points x_0, x_1, x_2, \dots in the phase space is called an “ ε -pseudo-orbit” or a “chain” of f if $d(f(x_i), x_{i+1}) < \varepsilon$ for every i . Computer-generated orbits, for example, are pseudo-orbits due to round-off errors. A fact of consequence to people performing numerical experiments is that in hyperbolic systems, small errors at each step get magnified exponentially fast. For example, if the expansion rate is 3 or more, then an ε -error made at one step is at least tripled at each subsequent step, that is, after only $O(|\log \varepsilon|)$ iterates, the error is $O(1)$, and the pseudo-orbit bears no relation to the real one. There is, however, a theorem that says that every pseudo-orbit is “shadowed” by a real one. More precisely, given a hyperbolic set, there is a constant C such that if x_0, x_1, x_2, \dots is an ε -pseudo-orbit, then there is a phase point z such that $d(x_i, f^i(z)) < C\varepsilon$ for all i . Thus, paradoxical as it may first seem, this result asserts that on hyperbolic sets, each pseudo-orbit approximates a real orbit, even though it may deviate considerably from the one with the same initial condition.

The shadowing orbit corresponding to a bi-infinite pseudo-orbit is, in fact, unique. From this, one deduces easily the following Closing Lemma: For any hyperbolic set, there is a constant C such that the following holds: Every finite orbit segment $x, f(x), \dots, f^{n-1}(x)$ that nearly closes up, that is, $d(x, f^n(x)) < \varepsilon$ for some small ε , lies within $< C\varepsilon$ of a genuine periodic orbit of period n . Thus, hyperbolic sets contain many periodic points.

Examples

Anosov Diffeomorphisms

A large class of Anosov diffeomorphisms comes from “linear toral automorphisms,” that is, maps of the n -dimensional torus induced by $n \times n$ matrices with integer entries, $\det = \pm 1$, and no eigenvalues of modulus one. The most popular example is the map obtained from

$$\begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix}$$

sometimes called the Arnol’d cat map because of an illustration used by Arnol’d. The unstable manifolds are lines parallel to the expanding direction shown in Figure 1 and wrapped around the torus, and the stable manifolds are obtained from the orthogonal lines.

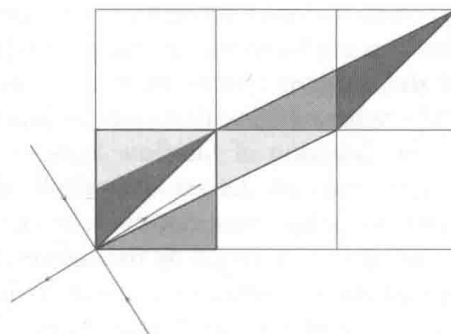


Figure 1 A hyperbolic toral automorphism. Reproduced from Katok A and Hasselblatt B (2003) *Dynamics: A First Course*. Cambridge: Cambridge University Press, with permission from Cambridge University Press.

We remark that due to their structural stability, (nonlinear) perturbations of linear toral automorphisms continue to have the Anosov property. This remark applies also to all of the examples below. In fact, all known Anosov diffeomorphisms are topologically identical to a linear toral automorphism (or a slight generalization of these, infranil-manifold automorphisms).

Geodesic Flows

Geodesic flows describe free motions of points on manifolds. Let M be a manifold. Given $x \in M$ and a unit vector v at x , there is a unique geodesic starting from x in the direction v . The geodesic flow φ^t is given by $\varphi^t(x, v) = (x', v')$ where x' is the point t units down the geodesic and v' is the direction at x' . Geodesic flows on manifolds of strictly negative curvature are the main examples of Anosov flows. They were studied by Hadamard (ca. 1900), Hedlund and Hopf (1930s) considerably before Anosov theory was developed.

Horseshoes

Smale’s horseshoe is the prototypical example of a hyperbolic invariant set. This map, so called because it bends a rectangle B into the shape of a horseshoe and puts it back on top of B , is shown in Figure 2. The set $\{x: f^n(x) \in B \text{ for all } n=0, \pm 1, \pm 2, \dots\}$ is hyperbolic. It is a two-dimensional Cantor set in B . The emergence of this example can be traced back directly to real-world systems.

During World War II, Cartwright and Littlewood worked on relaxation oscillations in radar circuits,

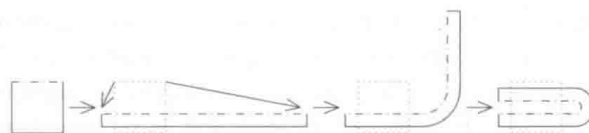


Figure 2 The horseshoe.

consciously building on Poincaré's work. Further study of the underlying van der Pol equation by Levinson contained the first example of a structurally stable diffeomorphism with infinitely many periodic points. (Structural stability originated in 1937 but began to flourish only 20 years later.) This was brought to the attention of Smale. Inspired by Peixoto's work, who had carried out such a program in dimension 2, Smale pursued a program of studying diffeomorphisms with a view to classification (Smale 1967). Until alerted by Levinson, Smale conjectured that only Morse–Smale systems (which have only finitely many periodic points with stable and unstable sets in general position) could be structurally stable. He eventually extracted the horseshoe from Levinson's work. Smale in turn was in contact with the Russian school, where Anosov systems (then C - or U -systems) had been shown to be structurally stable, and their ergodic properties were studied by way of further development of the study of geodesic flows in negative curvature.

The appearance of horseshoes in mathematical models of real-world phenomena is quite widespread. Indeed, in a sense this is the mechanism for the production of chaotic behavior, at least in dimension 2. In disguise, one of the earliest appearances of this phenomenon occurred in the prize memoir of Poincaré, where homoclinic tangles gave a first glimpse at the serious dynamical complexity that can arise in the three-body problem in celestial mechanics. If the stable and unstable curves of a hyperbolic fixed point intersect transversely (as in Figure 3a), this engenders further such intersections and produces a complicated web of accumulations of loops or lobes of stable and unstable curves, as shown in Figure 3b. Homoclinic tangles always produce horseshoes by the Smale–Birkhoff theorem, illustrated by Figure 3c, so in trying to solve the three-body problem, Poincaré essentially discovered the possibility of nontrivial hyperbolic behavior (see Homoclinic Phenomena).

A related appearance of horseshoes in this context is in the work of Alekseev, who used their presence to show that capture of celestial bodies can indeed occur.

Solenoids

Finally we mention the solenoid, which is an example of an Axiom-A attractor (see Figure 4). Here the map f is defined on a solid torus $M = S^1 \times D_2$, where D_2 is a two-dimensional disk. It is easiest to describe it in two steps: first it maps M into a long thin solid torus, which is then put inside M

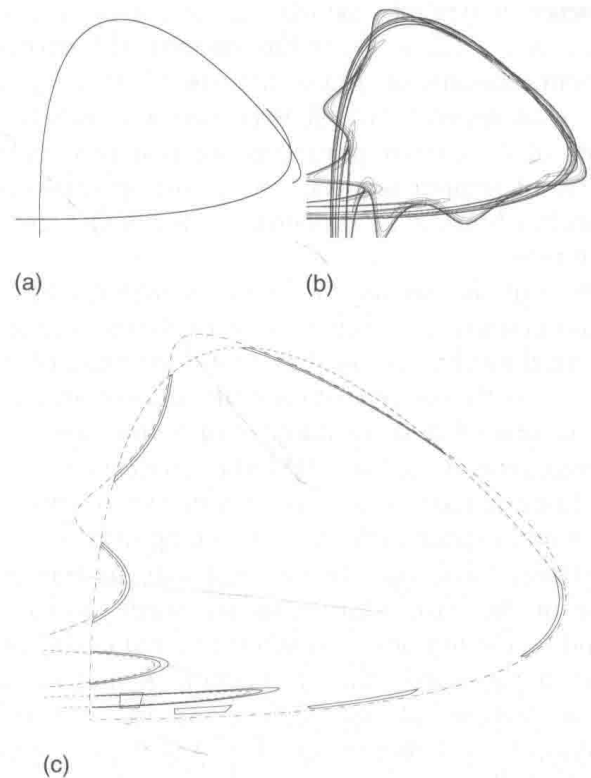


Figure 3 Homoclinic tangles produce horseshoes. Reproduced from Katok A and Hasselblatt B (2003) *Dynamics: A First Course*. Cambridge: Cambridge University Press, with permission from Cambridge University Press.

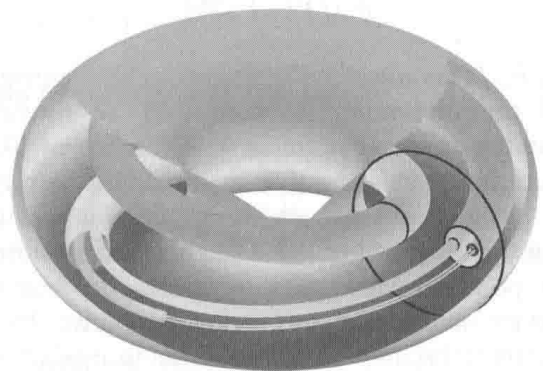


Figure 4 The solenoid. Reproduced from Katok A and Hasselblatt B (2003) *Dynamics: A First Course*. Cambridge: Cambridge University Press, with permission from Cambridge University Press.

winding around the S^1 direction twice. The attractor is given by $\Lambda = \bigcap_{n \geq 0} f^n(M)$.

Symbolic Coding of Orbits and Ergodic Theory

An important tool for studying the orbit structure of Axiom-A systems is the “Markov partition,” constructed for Anosov systems by Sinai and extended to Axiom-A basic sets by Bowen. Given a partition $\{R_1, \dots, R_k\}$ of the phase space, there is a natural way to attach to each point x in the phase space a

sequence of symbols, namely $(\dots, a_{-1}, a_0, a_1, a_2, \dots)$, where $a_i \in \{1, 2, \dots, k\}$ is the name of the partition element containing $f^i(x)$, that is, $f^i(x) \in R_{a_i}$ for each i . In general, not all sequences are realized by orbits of f . Markov partitions are designed so that the set of symbol sequences that correspond to real orbits has Markovian properties; it is called a shift of finite type.

The ergodic theory of Axiom-A systems has its origins in statistical mechanics. In a 1D lattice model in statistical mechanics, one has an infinite array of sites indexed by the integers; at each site, the system can be in any one of a finite number of states. Thus, the configuration space for a 1D lattice model is the set of bi-infinite sequences on a finite alphabet. Identifying this symbol space with the one coming from Markov partitions, Sinai and Ruelle were able to transport some of the basic ideas from statistical mechanics, including the notions of Gibbs states and equilibrium states, to the ergodic theory of Axiom-A systems.

The notion of equilibrium states, which is equivalent to Gibbs states for Axiom-A systems, has the following meaning in dynamical systems in general: given a potential function φ , an invariant measure is said to be an equilibrium state if it maximizes the quantity

$$h_\mu(f) - \int \varphi d\mu$$

where $h_\mu(f)$ denotes the Kolmogorov–Sinai entropy of f and the supremum is taken over all f -invariant probability measures μ . In particular, when $\varphi = 0$, this measure is the measure that maximizes entropy; and when $\varphi = \log |\det(df|_{E^u})|$, it is the Sinai–Ruelle–Bowen (SRB) measure. From the physical or observational point of view, SRB measures are the most important invariant measures for dissipative dynamical systems because if f is a diffeomorphism of a compact manifold M and Λ a transitive Axiom-A attractor with basin U , for example, $\Lambda = U = M$, then for Lebesgue-a.e. $x \in U$ and for every $\varphi \in C^0(M)$

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=0}^{n-1} \varphi(f^i(x)) = \int \varphi d\mu$$

that is, Lebesgue-a.e. point is μ -typical. Thus, while Axiom-A attractors will have chaotic motions, they are statistically coherent in that the asymptotic distribution of any typical orbit is given by the SRB measure.

Periodic Points and Their Growth Properties

We discuss briefly some further results related to the abundance of periodic points in Axiom-A systems.

For an Axiom-A diffeomorphism f , if $P(n)$ is the number of periodic points of period $\leq n$, then $P(n) \sim e^{bn}$, where b is the topological entropy of f . That is to say, the dynamical complexity of f is reflected in its periodic behavior. An analogous result holds for Axiom-A flows. This asymptotic behavior is known to remarkably fine accuracy (Margulis 2004), and these developments used the dynamical zeta function, which sums up the periodic information of a system. In the discrete-time case, $\zeta(z) := \exp \sum_{n=1}^{\infty} P(n)z^n/n$ has been shown to be a rational function analytic on $|z| < e^{-b}$. In the continuous-time case, the zeta function is given by $\zeta(z) := \prod_{\gamma} (1 - \exp(-zl(\gamma)))^{-1}$, where the product is taken over all (nonstationary) periodic orbits γ and $l(\gamma)$ is the smallest positive period of γ . This function is known to be meromorphic on a certain domain, but the location of its poles, which are intimately related to correlation decay properties of the system, remains one of the yet unresolved issues in Axiom-A theory.

Partial Hyperbolicity and Dominated Splitting

There are various ways in which the notion of hyperbolicity described above, which we will henceforth refer to as “uniform hyperbolicity,” can be extended beyond the one presented so far. This can be done with a view to weakening the conditions under which some of the salient properties of hyperbolic dynamical systems appear. The study of partially hyperbolic dynamical systems and that of dynamical systems possessing a dominated splitting is of this type. Further below, we describe a different extension motivated more by a desire to bring the results and methods of hyperbolic dynamics to bear on systems that are closer to some physical situations. This led to the study of nonuniformly hyperbolic dynamical systems.

If one views hyperbolicity as requiring that the spectrum of expansion and contraction rates is separated into two components by the unit circle, then one can consider systems where this separation is provided by a circle centered at 0 whose radius may not be 1 (partial hyperbolicity in the broad sense), or by two circles centered at 0 of which one has radius less than 1 and the other has radius greater than 1, with possibly a third component of the spectrum in the annulus between these (absolute partial hyperbolicity). Further weakenings are obtained by controlling not the whole spectrum in this absolute way, but rather ratios of expansion and contraction rates along orbits (dominated splitting

and relative partial hyperbolicity, respectively). Among the motivations for these weakenings are the desire to understand which systems are topologically transitive and robustly so (stable transitivity), and to understand which ergodic volume-preserving systems remain ergodic if perturbed within the space of volume-preserving systems (stable ergodicity).

Pseudohyperbolicity

Let f be a smooth invertible map. A compact invariant set of f is said to be partially hyperbolic in the broad sense if at every point in this set, the tangent space splits into a direct sum of two subspaces E^u and E^s with the property that these subspaces are invariant under the differential df , that is, $df(x)E^u(x) = E^u(f(x))$, $df(x)E^s(x) = E^s(f(x))$, and that there are constants $0 < \lambda < \mu$, $c > 0$ such that if $v \in E^s(x)$ for some x then $\|df^n v\| \leq c\lambda^n \|v\|$ for $n = 1, 2, \dots$ and if $v \in E^u(x)$ for some x then $\|df^{-n} v\| \leq c\mu^{-n} \|v\|$ for $n = 1, 2, \dots$. This is sometimes also referred to as the existence of a (λ, μ) -splitting or pseudohyperbolicity.

Dominated Splitting

A further weakening of this condition replaces these absolute estimates by relative ones. Let f be a smooth invertible map. A compact invariant set of f is said to admit a dominated splitting if at every point in this set, the tangent space splits into a direct sum of two subspaces E^u and E^s with the property that these subspaces are invariant under the differential and there are constants $\lambda \in (0, 1)$, $c > 0$ such that if $u \in E^u(x)$ and $v \in E^s(x)$ for some x then $\|df^n v\| / \|df^n u\| \leq c\lambda^n$ for $n = 1, 2, \dots$.

The presence of a dominated splitting has been found to yield substantial information pertinent to stability of such systems, and it plays a significant role in a program of research aiming at a classification of generic diffeomorphisms up to topological conjugacy and specifically motivated by the “Palis conjecture,” which aims to describe that classification. With respect to inferring topological and ergodic (i.e., statistical) properties of the orbit structure, the stricter notion of partial hyperbolicity (in the narrow sense below) is more commonly used, but in this respect the presence of a dominated splitting is also of interest because there is evidence in support of the conjecture that stable ergodicity implies the presence of a dominated splitting.

Partial Hyperbolicity

Let f be a smooth invertible map. A compact invariant set of f is said to be (absolutely) partially hyperbolic if at every point in this set, the tangent

space splits into a direct sum of unstable, central, and stable directions E^u, E^c , and E^s with the property that these subspaces are invariant under the differential df and that there exist numbers $C > 0$,

$$0 < \lambda_1 \leq \mu_1 < \lambda_2 \leq \mu_2 < \lambda_3 \leq \mu_3 \quad [1] \\ \text{with } \mu_1 < 1 < \lambda_3$$

such that if $v \in E^s(x)$, $w \in E^c(x)$, $u \in E^u(x)$, $n = 1, 2, \dots$, then

$$C^{-1} \lambda_1^n \|v\| \leq \|d_x f^n(v)\| \leq C \mu_1^n \|v\| \\ C^{-1} \lambda_2^n \|w\| \leq \|d_x f^n(w)\| \leq C \mu_2^n \|w\| \\ C^{-1} \lambda_3^n \|u\| \leq \|d_x f^n(u)\| \leq C \mu_3^n \|u\|$$

In this case, we set $E^{cs} := E^c \oplus E^s$ and $E^{cu} := E^c \oplus E^u$. Following Burns–Wilkinson, we say that f is “center-bunched” if $\max\{\mu_1, \lambda_3^{-1}\} < \lambda_2 / \mu_2$.

As in the case of (uniformly) hyperbolic dynamical systems, the sub-bundles E^s and E^u are integrable to stable and unstable foliations W^s and W^u . It is not automatic that the center-stable sub-bundle E^{cs} and the center-unstable sub-bundle E^{cu} are tangent to foliations W^{cs} and W^{cu} ; if this happens to be the case, the partially hyperbolic system is said to be “dynamically coherent.”

Partial hyperbolicity can also be defined by a cone criterion, with suitable adaptations.

Stable Ergodicity and Transitivity

Partial hyperbolicity was introduced as a means of providing just enough hyperbolicity to render a dynamical system ergodic or topologically transitive. These are both irreducibility conditions, and to obtain these, one rules out a Cartesian product situation by assuming something like essential accessibility: almost every two points (in the sense of volume viewed as a measure) can be connected by a curve consisting of a finite concatenation of arcs, each of which lies entirely in one stable or unstable leaf. A celebrated result in this field is in its original form (with a much stronger center-bunching assumption) due to Pugh and Shub: suppose a volume-preserving diffeomorphism is partially hyperbolic on the entire manifold. If it is dynamically coherent and center bunched and has essential accessibility, then it is ergodic (Hasselblatt and Pesin 2006).

One of the motivating aims of this theory was to obtain nonhyperbolic volume-preserving systems that are stably ergodic, that is, for which all volume-preserving C^1 -small perturbations are also ergodic. If, in addition to the above, one assumes that essential accessibility also persists under such

perturbations and that the center bundle E^c is integrable to a center foliation W^c that is smooth (or “plaque-expansive”), then ergodicity is indeed stable (Hasselblatt and Pesin). There are quite a few natural examples where these assumptions hold.

While essential accessibility does not always hold, it is fairly common. The stronger property of accessibility (that any two points can be connected, not only almost every two points) is conjectured to be stable under C^1 -perturbations and has been shown to hold for an open dense set of partially hyperbolic systems with respect to the C^1 -topology.

Ergodicity is a measure-theoretic irreducibility notion, and topological transitivity is the topological counterpart. It can also be obtained from accessibility: a partially hyperbolic volume-preserving diffeomorphism with the accessibility property is topologically transitive (in fact, almost every orbit is dense).

There are interesting converse results as well. Any stably transitive diffeomorphism exhibits a dominated splitting. Moreover, in dimension 2 it is hyperbolic and in dimension 3 it is partially hyperbolic in the broad sense.

Nonuniform Hyperbolicity

Applications have motivated weakening assumptions of uniform hyperbolicity to require only that “many” individual orbits exhibit hyperbolic behavior, without assuming that there are any uniform estimates on the degree of hyperbolicity.

To measure the asymptotic contraction or expansion of a vector on an exponential scale, one defines the Lyapunov exponent of a (nonzero) tangent vector v at x for the map f to be

$$\lambda(x, v) := \lim_{n \rightarrow \infty} (1/n) \log \|Df^n(v)\| \quad [2]$$

whenever this limit exists. Note that being positive indicates asymptotic expansion of the vector, whereas negative exponents correspond to contracting vectors. This defines a measurable but, save for exceptional circumstances, discontinuous function of x and v . It is relatively easy to see that for a given point x the function $\lambda(x, \cdot)$ can only take finitely many values, so it is natural to define nonuniform hyperbolicity as the property of having all of these finitely many values nonzero for “most” points. Given that λ is measurable, it is natural to define “most” by using a measure that is invariant under the map f . Therefore, the theory of nonuniformly hyperbolic dynamical systems, much of which is due to Pesin, is based on measure theory throughout.

The fundamental fact on which this theory is based is the “Oseledec’s multiplicative ergodic theorem,” which says that for a C^1 -diffeomorphism of a compact Riemannian manifold the set of Lyapunov-regular points has full measure with respect to any f -invariant Borel probability measure.

For a Lyapunov-regular point the limit [2] exists for all v , so this theorem tells us that no matter which invariant measure we consider, the limit [2] makes sense for all tangent vectors at points x outside a null set. (One should add that this small “bad” set can be somewhat substantial; for example, its Hausdorff dimension is usually that of the whole space.)

Accordingly, one then defines a measure to be hyperbolic if at almost every point the limit [2] is nonzero for all vectors. In this case, one says that “ f has nonzero Lyapunov exponents.” This property can also be obtained from a cone criterion, but here the family of cones may only be invariant and eventually strictly invariant, that is, there is a cone field such that cones are mapped to cones (but not necessarily into the interior of cones), and for almost every point there is an iterate that maps a cone strictly inside the cone at the image point (i.e., into the interior). Which iterate is needed is allowed to depend on the point (see Hyperbolic Billiards).

It is good to keep in mind that a hyperbolic measure may be concentrated on a single point, say, in which case there is not much gained by this approach. The theory is of great interest, however, if the measure is equivalent to volume or is the “physical measure” on an attractor.

Examples of this sort are fairly common, indeed any smooth compact Riemannian manifold other than the unit circle admits a volume-preserving Bernoulli diffeomorphism with nonzero Lyapunov exponents (Dolgopyat and Pesin 2002) (and every compact smooth Riemannian manifold of dimension at least 3 carries a volume-preserving Bernoulli flow for which at almost every point the only zero Lyapunov exponent is the one in the flow direction (Hu *et al.* 2004)).

Structurally, these systems exhibit many of the features seen in uniformly hyperbolic ones (e.g., stable manifolds), but instead of being continuous these are now measurable. There are, however, (noninvariant) sets of arbitrarily large measure on which these structures are continuous. This provides a handle for pushing some of the uniform theory to this context.

There are some topological results in this area, of which one of the more remarkable ones is that any surface diffeomorphism with positive entropy contains a horseshoe. Much of the current research is

directed at the ergodic theory of these systems. A central result from the initial development of the theory is that while these systems may not be ergodic, the ergodic components are (a.e. equal to) open sets, so in particular there are at most countably many of them.

One natural question is whether nonuniformly hyperbolic systems have SRB measures, and it is answered on a case-by-case basis. There are even benign examples where this fails to be the case, but for some realistic systems, such as the Lorenz and Hénon attractors, this has been established.

Because they preserve volume, this is not an issue for billiard systems, (*see* Hyperbolic Billiards), that is, the free motion of a point mass in a cavity with elastic boundary collisions. This describes not just a toy model, but also the phase space and dynamics of a gas of convex rigid bodies. Such a gas of hard spheres in a rectangular box is semidispersing and has been studied intensely. It is now known to be hyperbolic and hoped to be ergodic. (The latter would provide a solid foundation for statistical mechanics, at least for the case of spherical molecules.) A gas of nonspherical convex rigid bodies is also a point billiard, but it is not semidispersing, which puts it beyond the range of readily available techniques for establishing ergodicity.

Further Remarks

The historical remarks made here are significantly expanded in Hasselblatt (2002), which contains some references to yet more detailed sources as well as more detail about uniformly hyperbolic dynamical systems in a concise form. A concise but reasonably comprehensive and current account of partially hyperbolic dynamics is in Hasselblatt and Pesin, and an authoritative full presentation is in Pesin (2004). A survey of nonuniformly hyperbolic dynamics is given in Barreira and Pesin (2006), and the definitive treatment is given by Barreira *et al.*. A textbook presentation of (not only) hyperbolic dynamics is in Katok and Hasselblatt (1995) as well as Hasselblatt and Katok (2003), and much current research, including on all subjects discussed here, is surveyed in Handbook.

See also: Ergodic Theory; Fractal Dimensions in Dynamics; Generic Properties of Dynamical Systems; Homoclinic Phenomena; Hyperbolic Billiards; Inviscid Flows; Lyapunov Exponents and Strange Attractors; Regularization for Dynamical Zeta Functions; Singularity and Bifurcation Theory; Symmetry and Symmetry Breaking in Dynamical Systems.

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世

界著名数学家、哲学家、逻辑学家弗雷格曾给出了一个著名等式：半个数学家+半个哲学家=好的哲学家+好的数学家。他解释说：“一个好的数学家，至少是半个哲学家；一个好的哲学家，至少是半个数学家。”

本书的目的就是要用物理学家替换上述等式中的哲学家。

举两个刚刚读到的例子，从中可见物理学家对数学也会有贡献。物理学家李政道和杨振宁在研究统计力学的一个问题时，遇到了一类特殊的多项式

$$P(z) = \sum_{j=0}^{\infty} a_j z^j$$

的集合 \mathcal{P} 。他们能够分析出， \mathcal{P} 中的任意一个多项式 P 的所有根都位于复平面的单位圆周 $\{z: |z|=1\}$ 上。因此他们猜测这个结论对 \mathcal{P} 中的所有多项式 P 都成立。如果他们可以找到一个酉矩阵 U 使得 $P(z)$ 是 U 的特征多项式，即 $P(z) = \det(zI - U)$ ，那么猜想就证明了。这是任何一个学过高等数学的人都会想到的办法，但这个方法在此不管用。杨和李有很好的数学功底，因此找到一个证明，但这个证明并不简单。现在有更容易的证明了，这要特别归功于浅野太郎 (Taro Asano)。为证明杨-李单位圆定理 (将在下面陈述)，我们需要将单变量 z 的 m 次多项式 P 替换为 m 个变量 z_1, \dots, z_m 的多项式 $Q(z_1, \dots, z_m)$ ， $Q(z_1, \dots, z_m)$ 关于每个变量 z_i 都是一次的。我们感兴趣的是这样一类多项式 $Q(z_1, \dots, z_m)$ 的集合 \mathcal{Q} ：只要 $|z_1| < 1, \dots, |z_m| < 1$ 就有 $Q(z_1, \dots, z_m) \neq 0$ 。因此，如果 $P(z) = Q(z, \dots, z)$ 且在 \mathcal{Q} 中，则 P 的根 ξ 满足 $|\xi| \geq 1$ 。(在我们感兴趣的情况下，存在一个对称 $z \rightarrow z^{-1}$ ，因此也有 $|\xi^{-1}| \geq 1$ ，从而 $|\xi| = 1$ 。) 很明显，如果 $Q(z_1, \dots, z_m)$ 与 $\tilde{Q}(z_{m+1}, \dots, z_{m+n})$ 在 \mathcal{Q} 中，则

$$Q(z_1, \dots, z_m) \tilde{Q}(z_{m+1}, \dots, z_{m+n})$$

也在 \mathcal{Q} 中。我们现在描述一个不那么显然的运算，称之为浅野缩并，它将 \mathcal{Q} 中的多项式变为 \mathcal{Q} 中的多项式。记

$$Q(z_1, \dots, z_m) = Az_j z_k + Bz_j + Cz_k + D$$

其中 A, B, C, D 是变量 z_1, \dots, z_m 中除去 z_j, z_k 之外的其余 $m-2$ 个变量的多项式。浅野缩并将两个变量 z_j, z_k 替换为一个单独的变量 z_{jk} ，使得

$$Az_j z_k + Bz_j + Cz_k + D \rightarrow Az_{jk} + D$$

从一个 m 元多项式 Q 出发，经过一次浅野缩并，我们得到一个 $m-1$ 元多项式，如果原来的多项式在 \mathcal{Q} 中，则所得的新的多项式也在 \mathcal{Q} 中。(这是一个简单的练习： $Az_{jk} + D$ 的根是 $Az^2 + (B+C)z + D$ 的两根之积的相反数。) 可以验证，如果 $-1 \leq a_{jk} \leq 1$ ，则两个变量 z_j, z_k 的形如

$$z_j z_k + a_{jk} (z_j + z_k) + 1$$

的多项式也在 Q 中。(令多项式等于零, 则得到一个映射 $z_j \rightarrow z_k$, 该映射是一个对合, 并且将单位圆的内部映射到单位圆的外部。) 将这些多项式相继相乘, 当同一个变量出现两次时做一次浅野缩并, 最后令所有的变量都等于 z , 则我们得到杨—李单位圆定理: 对于实数 $a_{jk} = a_{kj}$, $-1 \leq a_{jk} \leq 1$, 多项式

$$P(z) = \sum_{X \subset \{1, \dots, m\}} z^{|X|} \prod_{j \in X} \prod_{k \notin X} a_{jk} \quad (*)$$

的所有根都位于单位圆周上^①。

再比如物理学家张宗燧。张宗燧步入量子场论研究领域, 主要受到玻尔(N. Bohr)的影响。从两人的通信中, 可以看出张宗燧对理论研究的偏好。而在理论研究中, 张宗燧又有明显的数学倾向。其研究特点为: 数学技巧强, 善于应用数学解析物理理论问题。在物理研究中, 他主张多做群论和对称性的工作。其研究成果中数学计算和表达都相当“清楚、干脆、可靠”, 结论简明准确。在《数学译林》为田方增先生百岁诞辰的贺信中就提到: 泛函分析学科在中国科学院数学研究所几乎一开始就是基础理论与应用并重地发展。按科学规划的精神, 从1958年起数学所泛函分析学科强调其发展要侧重于与微分方程、物理学、高尖科技和国民经济建设之联系。为此, 田方增、关肇直常与吴新谋、张宗燧等合作, 使数学所内泛函分析的发展始终注意与微分方程及现代数学物理的联系, 先后组织了量子场理论、粒子迁移理论和电磁波理论中数学问题之研究等学术讨论班。他撰写的学术论文为发展中国在这一领域的数学研究做出了重要贡献。田方增与关肇直一起成功地在中国开辟了应用泛函分析的一个重要领域——粒子迁移理论的数学基础及问题的研究。

所以说数学和物理互易性强。一些数学家后来成了物理学家(例如戴森(Freeman Dyson)), 而另一些人正好相反(例如钱德拉(Harish Chandra)、博特(Roul Bott)), 他们从物理学家变成了数学家。最夸张的莫过于威腾(Edward Witten, 1951—), 1990年获得菲尔兹奖的理论物理学家威腾于1976年在普林斯顿大学在诺贝尔奖得主(2004)格罗斯(David Gross)的指导下获得物理学博士学位; 但他从未获得过数学博士学位。

那么学习物理到底应该掌握多少数学呢?

一位致力于学习理论物理的学生曾请教赫柏林院士怎样治学。赫先生说: “要想搞理论物理, 首先数学要好。前两年先把斯米尔诺夫的五卷及变分学、微分几何、数理方法、拓扑和积分等学完, 然后开始进入近代数学, 要学流形、群、连续群、李群、现代微分几何等。”

当然这只是入门级的数学。

本套丛书貌似物理实则充斥着现代数学, 正如中国科学院理论物理研究所吴岳良研究员所评介的那样:

本书物理学部分与数学部分的关系很难分开。实际上, 经典力学、电磁学、统计力学、量子力学、流体力学、可积系统和动力系统许多物理问题可归结为求解数学上的常微分方程、偏微分方程、积分方程、微分积分方程等数学物理方程, 物理学问题的解会涉及复变函数和特殊函数等多种函数, 在求解时又会用到变分技术、调和分析、泛函分析等各种数学分析方法。同时, 对爱因斯坦狭义相对论和广义相对论, 它不仅改变了人们的时空观, 还使得闵可夫斯基时空的几何学和黎曼空间的几何学成为物理理论的数学基础, 同时也使得向量分析、张量分析和微分几何等成为必要的数学分析工具。在量子力学中, 物理量成为算子, 物理状态用波函数来描述, 算子的谱才是测量到的物理量。在量子场论中, 波函数又被二次量子化成为算子用来描述基本粒子在相互作用过程中的产生和湮灭。这使得算子代数、量子化方法和路径积分等数学理论和方法成为量子物理的数学基础。粒子物理学家发现自然界的3种基本作用力: 电磁相互作用、弱相互作用和强相互作用可用规范理论来描述, 并完全由规范对称性来支配, 这些对称性在数学上用李群和李代数来描写。事实上, 晶体的结构也是由欧几里得空间中的转动群来描述, 这使得群论在物理学中的应用, 尤其在粒子物理中的应用变得越来越重要。在规范理论中, 规范势当作基本的量子场, 而它被发现就是数学家在现代微分几何学中所研究的纤维丛上的联络, 这使得有关纤维丛的拓扑不变量在粒子物理和量子场论研究中变得重要起来, 如规范场的磁单极子和瞬子解及手征量子反常等。在量子引力和超弦理论的研究中, 不仅运用到已有的数学理论和方法, 尤其是现代数学, 还促进了数学理论本身的发展。同样, 在凝聚态物质和光学方面, 物质的拓扑相和拓扑缺陷、拓扑量子计算等也应用到了许多现代数学方法, 这使得代数拓扑、代数方法、量子群、复几何、辛几何与拓扑、低维几何、非交换几何等数学理论和数学方法越来越多地渗透到理论物理的研究中。另外, 在研究微观物理对象的随机性和各种随机过程的统计规律、无序系统和动力系统时, 随机方法和离散数学等也得到越来越广泛

① 见杨振宁, 李政道, “Statistical Theory of Equations of State and Phase transition. II. Lattice Gas and Ising Model”, Phys. Rev. (2) 87(1952), 410-419; 也见 T. Asano, “Theorems on the partition functions of the Heisenberg ferromagnets”, J. Phys. Soc. Japan, 29 (1970), 350-359. 长期以来我都为杨—李单位圆定理着迷(见 D. Ruelle, “Extension of the Lee-Yang circle theorem”, Phys. Rev. Lett. 26 (1971), 303-304), 而且我认为在这个领域仍然有未被揭示出的神秘。(2010年, 吕埃勒再次发表了一篇关于杨—李单位圆定理的文章, 见 Characterization of Lee-Yang polynomials, Annals of Mathematics, 171(2010), 589-603. ——译者注。)

的应用。

数学对物理的影响有多大？

正如本书前言中所写：

当然，数学是确实存在的。事实上，从某种角度而言，物理学是由精确的数学逻辑所操控的：古希腊人把空间几何结构变成了一种真实的艺术形式。就我所知，古希腊人是“数学物理”的第一个践行者，他们引入了坐标轴的概念，从而把空间几何的所有量都转化为一些简单的数字。今天，这些被称作“物理学的基本定律”，直到很久以后我们才认识到如下事实：时间流可以类似地被坐标化，它连同空间一起，同样可用几何方法来解决。于是，有一些疯狂的人对数字的魔力很感兴趣，但是，我们的现实世界似乎确实包含许多超出我们分析能力的地方。

渐渐地，所有这一切都变了。月亮和其他行星的运动好像都满足几何定律。伽利略和牛顿设法去发现这些运动的合乎逻辑的定律，并注意到质量的概念也适用于太空中的物体，就像地球上的苹果和大炮一样，这使得太空更容易被我们所理解。同时人们发现，电子、磁场、光和声音也完全按照数学方程在运转。

科学家认为：开展对“数学物理”的深入研究，有助于揭示出物理学与数学之间的内在联系。事实上，从自然哲学发展到物理学，除了使用实验手段和新的思维方法，数学起了不可替代的作用。当人们通过分析大量实验数据和吸取各种唯象理论的精髓，以严格的数学语言和简洁的数学公式描述支配物质基本结构和宇宙演化的物理规律时，物理学的简洁美、统一美、对称与不对称美则通过深刻的数学美反映出来。可以说，自从物理学成为自然科学的一门独立学科后，物理学与数学之间的关系变得密不可分。古代的许多科学家既是数学家也是物理学家，尤其到了近代和现代，许多理论物理学家对数学的运用和发展起到了更为积极的推进作用，数学家和理论物理学家之间的合作也变得越来越频繁、越来越深入，他们成为了“数学物理”的践行者。大家最为熟知的古希腊的阿基米德，他既是著名的数学家也是著名的物理学家，他很早就利用数学这个工具证明了杠杆原理和浮力原理，并做了大量的实验。牛顿在研究物体和天体的运动规律时发展出新的数学方法——微积分。爱因斯坦则运用对当时的物理学家来说全新的数学方法——微分几何和黎曼几何，创立了广义相对论。爱因斯坦曾回忆说：“1912年我突然认识到，高斯的曲面理论是解开这个秘密的钥匙，他的曲面坐标系意义重大。不过，当时我还不不知道黎曼已经更深入地研究了几何基础。我突然想起，读大学时盖泽先生给我们上的几何就包括高斯理论……我认识到几何基础具有物理学意义。当我从布拉格回到苏黎世时，我亲爱的朋友、数学家格罗斯曼也在苏黎世。他告诉了我高斯，然后是黎曼。格罗斯曼两肋插刀，直接催生广义相对论。”

伟大的几何学家海曼·格拉斯曼^①在1844年发表的《Lineale Ausdehnungslehre》（《延拓理论》）。这本书像麦比乌斯的那本名著一样具有丰富的思想，但与麦的写作风格不同，非常晦涩，以至几十年未被人注意，也没有被人读懂，只是在其他书和文章中出现了一系列类似的思想之后，才认识到这些思想出自格拉斯曼的书，不过为时已晚。如果你想领略一下这种抽象的笔法，你只要看一下这本书里的某几章的标题，如：“纯数学之概念之导出”“延拓理论之推导”“延拓理论之叙述”“表示之形式”“一般形式理论之概述”，你只有费劲地钻通了这些内容之后才接触到所述内容的纯抽象的表示，不过仍然很难读懂。直到1862年该书出版了后期的修订本^②，格拉斯曼才用了一种比较容易接受的表示法，即坐标表示法。此外，格拉斯曼选了一个词——Ausdehnungslehre（延拓论），用以暗示他的研究可应用于任意维空间，而几何学对他而言只不过是这个完全抽象的新学科在普通三维空间中的应用。但是他造的这个新词并没有生根，人们现今简称为“ n 维几何学”。

我们普通读者可能易将数学物理与数学物理方程相混淆，其实这是两个内涵和外延都不同的概念，后者只能视为前者的一个真子集，而前者不论从内容上还是所涵盖的范围都远远超过了后者，但有一点共同之处是它们的问题都源自于物理，但解决都来自于数学家。比如迪利克雷猜想的解决，“迪利克雷原理”这一数学猜想自提出之日起，历经了三十多年的激烈论争和反复，最终才被确立，这是迪利克雷在研究微分方程位势原理时提出的一个猜想，其具体内容简单地说大体是：极小化迪利克雷积分

$$\iint \left\{ \left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial u}{\partial y} \right)^2 \right\} dx dy$$

的函数 u ，满足位势方程

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$$

① 海曼·格拉斯曼，《延拓理论》出版于1844年莱比锡。并可参阅其 Gesammelte mathematische und physikalische Werke，第1卷，莱比锡，1894年，第二版出版于1898年莱比锡。

② 柏林，1862年。见其著作集第1卷第二部分，莱比锡，1896年。

后来有人在研究三维位势方程(亦称拉普拉斯方程或调和方程)

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = 0$$

时,又提出,由位势方程所描述的相应物理状态总有一个确定的物理解,因而其本身也必然存在一个数学解,但在数学上的这种存在性,长时间的不能被证明,直到1851年,黎曼才在他的博士论文“单复变函数一般理论的基础”中,给出了位势方程边界问题解的存在性证明.由于黎曼在文中运用了他的老师迪利克雷所提出的上述猜想,故他称之为“迪利克雷原理”.可是,在其论文发表后的不长时间,这个原理便激起了热烈的讨论,特别是黎曼的这一证明受到了德国著名数学家魏尔斯特拉斯(K. W. Weierstrass, 1815—1897)的尖锐批评,他指出:黎曼不加证明就先验地假定一定会存在一个使积分取得到极小值的函数,这在数学上是不允许的,尽管受到了大师的批评,黎曼并没有因此动摇自己对迪利克雷原理的信心,并且一鼓作气又运用此原理作出了一系列重要的发现.1866年,黎曼英年早逝,但关于迪利克雷原理是否成立的争论仍未停止.1870年,魏尔斯特拉斯给出了一个与迪利克雷原理相反的例子,在这个例子中,对给定的边界条件,使迪利克雷积分达到极小值的函数是不存在的,并以此来否定迪利克雷原理.由于迪利克雷原理被当时的数学权威魏尔斯特拉斯所否定,所以数学家们只好另辟蹊径来证明位势方程边界问题解的存在性,比较著名的有三种证法,1870年纽曼用“算术平均值法”给出了一个证明;1890年,许瓦兹用“交替法”又给出了一个证明,同年,庞加莱用“扫散法”也给出了一个证明.这些证明从逻辑上讲无疑都是对的,但就是没有一个能够像以迪利克雷原理为工具那样简单、明快,这又不禁使得数学家们怀念起“迪利克雷原理”来,都对它当年被否定而感到惋惜,并随之产生了复活这一原理的念头,并且也为之做出了一些努力,只可惜都未能成功,数学界为此弥漫着一种悲观的气氛,数学家纽曼就表示:如此优美而又有如此广阔应用前景的迪利克雷原理,已经从我们的视线中“永远消失”掉了!

俗话说“三十年河东,三十年河西”,就在迪利克雷原理被否定三十年之后,即1899年,德国领袖数学家希尔伯特对此又发动了一场新的“救亡运动”.他彻底冲破了那种把严格性与简单性对立起来的传统观念,批判了魏尔斯特拉斯以严格性全盘否定迪利克雷原理的做法,从迪利克雷原理的简单性、优美性以及应用的有效性出发,积极寻求它的真实性和合理性,最后终于找到了证明迪利克雷原理的途径和方法,他在德国数学联合会上报告了他的这一研究成果,并明确指出:只要对问题中的区域、边界值和允许函数的性质作适当的限制,就完全可以恢复迪利克雷原理的真实性.他还针对数学家们认为迪利克雷原理早已沉没了的观点,意味深长地将他的这一研究工作称为“迪利克雷原理的复活”.后来希尔伯特又给出一个更为一般的证明,从而进一步肯定了迪利克雷原理存在的合理性.

及至近代更多源自于物理的数学理论被抽象出来,而对这些数学理论的进一步研究又极大地推动了物理学的进展,如Yang-Mills规范场的大范围整体性质和手征量子反常与纤维丛的拓扑不变量和Chern-Simons示性类及指标定理之间建立起直接的联系,超弦理论中的额外维空间与Calabi-Yan空间之间的对应关系.理论物理学家威滕在发展超弦理论的同时由于对数学的杰出贡献而获得菲尔兹奖,这些都是物理学与数学相结合所呈现在“数学物理”方面的经典例子.

对此我国数学工作者早有清醒的认识,20世纪80年代李大潜就撰文指出,学数学的追求纯而又纯的境界,即使从纯数学的发展来说,也不见得是一条康庄大道.不重视实际的需要和其他领域的发展,没有广阔的视野,是很难出第一流的基础理论人才的.

基础和应用有着密切的关系,而且相互促进.搞基础理论的人重视应用方面的教育和训练,对基础理论和应用的研究会带来很大的促进.物理学中的规范场和数学上的纤维丛概念有密切的联系.据杨振宁教授自己讲,他在美国请教了很多纤维丛方面的数学家,但他们讲的一套,他听不懂,双方始终谈不到一起去.只有到了复旦大学,听谷超豪教授用物理学家可以接受的语言,把这两者的关系讲得很清楚,杨振宁教授很高兴,并和谷超豪教授合作,在规范场的数学理论方面做出很多成绩,把这方面的理论进一步发展了.为什么能这样呢?谷超豪教授在念大学时,就选修了物理系四大力学的课程.作为一个数学家,他不仅在数学上有很高的造诣,而且在物理学方面也有很好的修养.

从本书的目录我们可以看出它包含了相当全面的数学内容.它们分别是:数学物理学导言、经典力学、流体动力学、可积系统、经典场论、共形与拓扑场论、量子场论、广义相对论、量子引力、弦论与M-理论、凝聚态物质与光学、量子信息与量子计算、量子力学、无序系统、动力系统、平衡态统计力学和非平衡态统计力学、代数技巧、李群和李代数、离散数学、量子群、随机方法、复几何、微分几何、低维几何、非交换几何、代数拓扑、辛几何与拓扑、常微分和偏微分方程、泛函分析和算子代数、量子化方法和路径积分、变分技术.

本书的三位主编在序言中写道:“数学物理把数学和物理学这两大学科的优势集中到一起,它们的关系是共同发展.一方面,它运用数学这一工具把不断增长的精确性和复杂性这些物理概念组织了起来;另一方面,物理学家为数学家提供了灵感的源泉.”同时,也正如诺贝尔物理学奖获得者荷兰Utrecht大学Gerard't Hooft教授在前言中指出:“物理世界与数学世界之间存在明显的重要区别.物理世界强调事实的‘真相’,无论‘真相’是什么,而数学是纯逻辑和纯推理的世界.在物理

学中,一个理论是否能被接受是由实验来最后决定的。物理学中的方法论也与数学不同。”

一个广大读者所关注的例子是天体物理学家霍金是否完美地解决了黑洞火墙悖论?起码现在还没有定论,只能算是给出了第三种可能的解释而已。尽管人们对于黑洞的具体性质还没有全部了解,但是它作为一种致密天体的存在早已没有争议,而黑洞火墙悖论的中心,仍然在于量子力学与广义相对论的矛盾。量子力学把黑洞的视界定义为一个神秘的、拥有巨大能量的火墙,广义相对论则拒绝承认在宇宙中存在这种神奇的火墙,认为黑洞视界只是一种数学上的存在而已。因此,要想真正解决黑洞火墙悖论,人类需要对自然界有更深刻的理解。霍金自己也承认,要想真正理解物质和信息最终从黑洞中逃脱的原理,最终需要人们把引力和自然界的其他作用力合而为一,这是一个困扰了物理学家们将近一个世纪的难题,至今仍然没有得到解决。作为人类现代文明的两块基石,广义相对论通过优美的数学形式描述宇宙,目前人们认为对它已经有足够深刻的理解,而量子力学则通过一种概率化的形式描述微观世界,它的内涵和基本规律仍然不为人知,就连量子力学的创立者尼尔斯·玻尔也说“没有人理解量子力学”。黑洞火墙悖论是这两种理论在宇宙深处的交锋,而交锋的结果,目前仍然无法预料。

本书在刚引进中国时曾有过一个12卷精装本,以内容划分是一种创新,这种事出版界常有。

中央文献研究室所编《毛泽东年谱(1949—1976)》(中央文献出版社,2014)皇皇6卷,是读者期待已久的一部大书。不贤者识其小,这里只摘抄一点儿关于图书装订的内容。1965年8月14日,毛泽东就印一批马列经典大字本问题指示周扬:“同意用照相放大胶印的办法。但请注意封面不用硬纸;大书(例如《唯物主义与经验批判主义》《反杜林论》)过去例作一卷或两卷,现应分装4卷或8卷,使每卷重量减轻。”印大字本,是因为老同志视力差;封面不用硬纸,就是不要硬精装,因其不方便单手握卷,躺着阅读;较厚的书应该多分几册(其实毛泽东推举的两本书都在500页以下)。总体而言,毛泽东对大字本的这些要求,都是以读者为本位,以方便阅读为目的的。有人说:当今出版界在装订方面,流行大开本、大厚本、无线胶订,以傻、大、黑、粗为尚,这种专门为难读者的精神,实在令人费解。

但笔者认为本书绝对算得上是数学物理中的经典之作。而向经典致敬的方式各有不同,最传统、最有效的就是保持原汁原味。原来我们准备连封面都拷贝原版,后与版权代理协商才改成现在的样子。真正美好的东西都一定是增一分则多,减一分则少,原来就刚刚好,我们为什么要破坏它呢?难道我们真的有自信会使其变得更好吗,佛头著粪与狗尾续貂都会让读者吐槽的。

还有一个原因使我们一定要保持原貌,那就是翻译的巨大工作量,我们哈尔滨工业大学出版社地处北方,远离经济与文化中心,实在是没有能力组织庞大的翻译队伍,耗巨资多年打磨这套丛书。我们待将来实力增强后再购买中文版权来完成这一宿愿。在购买版权时我们也表达了购买数字版权的意向,但被婉拒了,因为英文版的数字出版外方已做得很完善了,不像我们刚起步,而且在碎片化之后还面临着版权保护问题,在辞典出版中这是个顽疾。举个例子:

认不认得这个英文单词 esquivallence? 不认得? 那你可以去查一下新版的《新牛津美语词典》(《New Oxford American Dictionary》),里面会告诉你这个词的意思是:“故意逃避自己的官方责任。19世纪开始出现,或许是源自法文 esquiver,“躲避,溜走””。

不过如果你拿起家中案头的其他词典,或者将词输入到各种电子词典中,保证你怎么查都查不到这个词,要是你查到了,那可就有事了。

为什么会这样?因为这个词根本就是《新牛津美语词典》编辑部发明的,不存在的词。什么?词典里竟然有虚构的词?编词典的人怎么可以干这种事?

词典里有虚构的词,不只《新牛津美语词典》,基本上每一本词典里都藏有这种凭空创造的词,放这样的词在词典里,倒不是出于编辑的恶作剧坏心,而是有具体用处的。

这是保护著作权的重要机关。辛辛苦苦编出一本厚重的词典,要如何防止别人贪便宜,把你的词典拿去剪剪贴贴,改头换面就变出他们的词典呢?词是共通的,词的意思解释也不会有多大的差别,要怎样证明别人的词典抄袭、盗取你的内容?

要是 esquivallence 这个词出现在《新牛津美语词典》以外的词典里,就一定牵涉到抄袭、盗取,这个词就是为了找出抄袭、盗取而放在那里埋伏的。

当前全球出版业都不景气,特别是在纸书出版领域。中国出版业尤甚,凉意十足。尽管各路专家给出了不同的原因分析,但只有一位专家给出的答案令业内所信服,那就是优质内容的缺失。说到底出版是一个内容为王的产业,没有好的内容,一切都是无本之源。

有位作家说:平庸是这个时代的危险所在,它无法再吸收传统知识;现代生活杂乱无章,令人湮没无闻。一切都掉在浅水中,没有什么沉入深深的井中;一切都是飞短流长,一切都是流言蜚语。

我们应该敢于承认一个基本事实,这个事实便是——在这个平庸的时代,最坏的都活下来了,最好的死去了,我们这些还能逃生的,发挥不出真正的价值。那么,在这个平庸的时代,我们还能做什么呢?

由衷感谢爱思唯尔(Elsevier)公司于2006年6月出版的这套《Encyclopedia of Mathematical Physics》(《数学物理大百科全书》),这是一部不平凡的全面介绍数学物理知识的百科全书。

本书的三位主编(法国巴黎居里大学 Jean-Pierre Francoise 教授、美国费城德雷塞尔大学 Gregory L. Naber 教授和英国牛津大学 Tsou Sheung Tsun 博士)都是长期从事数学物理方面研究的知名学者,他们邀请了包括诺贝尔物理学奖获得者杨振宁教授和英国牛津大学 Roger Penrose 教授在内的34位著名物理学家和数学家,作为本书的编辑顾问委员会成员,组织来自30个国家的439位在物理学和数学相关研究领域做出杰出贡献的理论物理学家和数学家,撰写了400多篇图文并茂的综述性文章。

《数学物理大百科全书》是经长达4年完成的一部内容全面系统、领域涵盖广泛的百科全书,全书特色鲜明,既体现了学科的基础性、独立性、完整性,又注重学科的前沿性、交叉性、应用性,是当今数学物理研究领域最新和最全的百科全书。

本书内容涉及物理学和数学的几乎各个重要研究领域,遍及从经典力学到量子力学、经典场论到量子场论、共形场论到拓扑场论、流体动力学到动力系统、可积系统到无序系统、粒子物理到天体宇宙学、相对论到量子引力、规范理论到统一理论、平衡态统计到非平衡态统计、凝聚态物质到量子信息、变分技术到代数方法、泛函分析到算子代数、路径积分到随机方法、李群到量子群、微分几何到代数拓扑、低维几何到非交换几何、复几何到辛几何等核心领域和方向,本书还特别注重数学物理的最新研究成果和在各领域的最新应用,并提供了大量必要的和重要的参考文献。

本书相比一般的百科全书有一个明显的亮点是它的综述,它可以告诉你你所想知道的某个专题的一切。中国科学院院士赫柏林曾留学于哈尔科夫大学,据他回忆当时的考试是由数学物理教授 A. Ya. Povzner 主持,他出的题目是:“把从你生下来以后所知道的贝塞尔函数的一切都告诉我。”据他的学生说:他写了一大摞纸,密密麻麻,然后告诉 Povzner“这是我知道的关于贝塞尔函数知识的提纲。若是需要,我可以展开每一项的具体内容。”于是考试通过。

正如 Gerard't Hooft 所指出的那样:

数学物理这个交叉学科是非常难懂的,百科全书中的某些题目纯粹是物理的,高 T_c 超导电性、破坏水波和磁水动力是完全物理的题目,其中的实验数据比任何高深理论都具有决定性。然而,上同调理论、Donaldson-Witten 理论和 AdS/CFT 对应是纯数学的例子。

在编辑中,大量不同作者的短小文章不可避免地被做了适当的变动,在这本百科全书中,理论物理学家和数学家为高等数学物理中的许多重要条目做了简单明了的阐述,所有的文章都包含了供进一步阅读的参考文献,我们盼望这些努力会取得很好的效果。

本书的编者认为:

与狭义的数学和物理学的古老历史相比,数学物理是一门相对较新的独立学科,数学物理国际协会成立于1976年,当然,从古时候起数学与物理学就相互影响,但近几十年来,可能因为我们正身在其中,它们出现了巨大的进展,新的结果和观点以令人目眩的节奏诞生,以至于需要有一本百科全书来搜集整理这些知识。

数学物理把数学和物理学这两个大学科的优势集中到一起,它们的关系是共同发展,一方面,它运用数学这一工具把不断增长的精确性和复杂性这些物理概念组织了起来;另一方面,物理学家为数学家们提供了灵感的源泉,两者关系的经典例子是爱因斯坦的相对论,其中微分几何在物理理论的公式化方面起到了实质性的作用,而物理学相继提出的问题推动了微分几何的发展,巧合的是,当我们在为《数学物理大百科全书》写序言时,正值爱因斯坦创造奇迹100周年。

再三考虑到写这部《数学物理大百科全书》是一个艰巨的项目,如果不是坚信这是一项很有意义的、受益于社会的项目,而且我们会得到众多的支持,那么我们绝不会接受这个任务,我们确实获得了许多支持,包括建议、鼓励和有实用性的帮助,这些支持来自编辑顾问委员会成员和我们的作者,还有其他慷慨地抽时间帮我们完善这本百科全书的人。

数学物理是一门较新的学科,它还没有被清晰地刻画,不同的人对它有不同的理解,在我们选择的题目中,一部分遵循了近期数学物理国际大会的纲要,但主要参照编辑顾问委员会和作者的提议,由于时间和空间的限制,以及我们自身的水平所限,更改了某些冗长的题目,但我们尽量收录了我们认为是核心的课题,尽量覆盖更多的最活跃的领域。

近年在中国对本书的原出版商还是有些负面新闻的,起源是在美国一个名为“知识的代价”网站上,已有全球12196位科学家签名抵制这家世界上最大的出版商,有人用“学术之春”形容这场运动。

吹响号角的是大名鼎鼎的英国数学家威廉·提摩西·高尔斯(William Timothy Gowers),这位来自剑桥大学的菲尔兹奖得主曾发表了一篇博客文章,号召同行行动起来,抵制世界上最大的出版商爱思唯尔集团。

读到这篇博文的泰勒·内伦(Tyler Neylon)——一位目前在硅谷开公司的数学博士当即给高尔斯教授留了言,第二天,他建立了一个网站,命名为“知识的代价”。

泰勒事后回忆,自己读到那篇博文,就意识到可以做点什么,在他看来,高尔斯是一位拥有号召力的“超级明星”。

迄今为止,数万名科学家在泰勒的网站上签了名,他们发誓,不在爱思唯尔旗下的期刊发论文,不做审稿人,或者不担

任编辑。

尽管如此,我们还是选择了与爱思唯尔的合作,因为一套好的大百科太难得了。

旅法钢琴大师白建宇(Kun-Woo Paik)对钢琴的要求非常苛刻,他在一次与台湾出版人郝明义先生的谈话时说,弹琴弹到现在,职业演奏生涯超过半个世纪,所遇到满意的琴竟不超过5架,如此答案,令见多识广的郝先生也大吃一惊。

在数理方面,近年来国内引进的好的大百科也绝不会超过5部,前苏联五卷本的《数学大百科全书》算一部,日本岩波的《数学百科全书》算一部,总之是屈指可数。

其实这个项目并不是爱思唯尔创始的,据介绍,这个项目开始于 Academic Press,后来由爱思唯尔接手。他们热情的工作人员,把过渡工作做得天衣无缝。并且令人感动的是,相当一部分作者慷慨地把他们的酬劳捐赠给欧洲数学会的发展中国家委员会,我们应该感谢他们为发展中国家所做的一切。

至于我们最关心的问题:谁会去购买这样一套大书,我们充满乐观。大千世界无奇不有,各种购买方式都可能出现。前一阵子,有关霍金打赌输掉关于“上帝粒子”存在性的赌约报道很多。

实验证明霍金输掉了这场赌约,霍金坦承自己输得心服口服并祝愿希格斯获得诺贝尔奖。希格斯透露,在宣布发现新粒子后,霍金曾与他联系并表示支票已寄出。希格斯说,“他不仅是给我一个人钱,我想他还会寄100美元给密歇根大学的戈登·凯恩。”

这场赌约的另一位赢家凯恩对来自霍金的美元欣然接受。“我坚信希格斯玻色子一定会被找到,发现希格斯玻色子真是太棒了,它证实了长久以来的猜想,进一步加强了粒子物理‘标准模型’的事实根据,打赌获胜是锦上添花。”凯恩表示要把赢来的钱花在刀刃上,所有的钱都要用于搞研究。

霍金可能已经习惯了以输掉赌约的方式推进科学的普及。

1975年,霍金曾关于天蝎座X-1是否包含黑洞打赌,后来认输,为赢家订阅了1年的《阁楼》杂志。

1991年,霍金又与人赌上了,这次赌的是裸奇点是否存在,霍金再次输了。

第三次打赌发生在1997年,霍金同美国物理学家约翰·普雷斯基尔打赌,认为黑洞部不会摧毁它们吞噬的一切信息,霍金于2004年7月21日当众表示输掉了这场赌约,并送给普雷斯基尔一套板球百科全书。

关于希格斯玻色粒子的赌约则是他的第四场赌约。这30多年来,霍金通过杂志、书籍和一点点美元,让更多的人了解到这些科学最前沿的问题。在100美元的赌约背后,希格斯的远见和霍金的牺牲精神都值得称道。

我们期待下一个赌约会以这样一套百科全书来结束。

著名力学家周培源90岁生日时,北京大学全体师生用“献身科学,教育英才;功在国家,造福将来;寿齐嵩岱,德被春荻;祝嘏欢呼,潸欤盛哉”的贺词赞扬他们的老校长。斗胆借用一下,庆祝这套书在中国的出版,当不为过。

刘培杰

2015年11月1日

于哈工大



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